Electronic Supplementary Material (ESI) for RSC Advances.

Synthesis of 3-(5-amino-1*H*-1,2,4-triazol-3-yl)propanamides and their tautomerism

(Electronic Supplementary Information)

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Synthesis of starting materials (Experimental)

General

Melting points (uncorrected) were determined on a Stuart™ SMP40 automatic melting point apparatus. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker Fourier 300 spectrometer (300 MHz), using DMSO-d_6 as a solvent and TMS as an internal reference. IR spectra were recorded on a Varian 640-IR FT-IR spectrometer using KBr mode. Microwave-assisted reactions were performed in closed vessel focused single mode using a CEM Discover SP microwave synthesizer (CEM, USA). The reaction temperature was measured by an equipped IR sensor.

Synthesis of *N*-guanidinosuccinimide (2)

A mixture of aminoguanidine hydrochloride (6.6 g, 60 mmol) and succinic anhydride (6.6 g, 67 mmol) was heated in an oil bath until all solids melted. Reaction mixture was continuously stirred with a glass rod until the molten mixture solidified. Reaction mixture was heated for another 30 min. Solidified reaction mixture was then cooled to room temperature, followed by the addition of 10 mL of water and 27 mL of ethanol. The resultant mixture was refrigerated and the deposited solid was filtered and washed with ethanol. The crude solid was added to aqueous solution of sodium bicarbonate (3.5 M, 7 mL) and stirred for 20 min at room temperature. The product was filtered and washed with cold water and recrystallised from acetonitrile.

White solid; yield: 3.2 g (88%); mp > 350 °C (MeCN), lit.[1] > 300 °C.

^{1}H NMR (300 MHz, DMSO-d_6): δ 2.50 (4H, s, CH_2CH_2), 5.26 (2H, br s, NH_2), 5.60 (2H, br s, NH_2).

^{13}C NMR (75 MHz, DMSO-d_6): δ 26.7 (CH_2CH_2), 159.8 (N=C(NH_2)$_2$), 175.4 (2 x C=O).

***N*-arylsuccinimides 4b, 4e, 4g, 4j, and 4k); General Procedure**

A mixture of substituted aniline (2 mmol), succinic anhydride (300 mg, 3 mmol) and *N*,*N*-diisopropylethylamine (70 µL, 0.4 mmol) in tetrahydrofuran (1 mL) was irradiated in 10 mL seamless pressure vial using microwave system operating at maximal microwave power up to 300 W at 180 °C for 15 min. After cooling, the product was filtered and washed with tetrahydrofuran. Analytical sample was recrystallised from a suitable solvent.

***N*-(4-fluorophenyl)succinimide (4b)**

White solid; yield: 217 mg (56%); mp 172-173 °C (MeOH), lit.[2] 175-177 °C.

^{1}H NMR (300 MHz, DMSO-d_6): δ 2.77 (4H, s, CH_2CH_2), 7.31-7.33 (4H, m, H-2', H-3', H-5' and H-6').

^{13}C NMR (75 MHz, DMSO-d_6): δ 28.4 (CH_2CH_2), 115.6 (d, $^{2}J_{CF}$ = 22.9 Hz, C-3' and C-5'), 128.9 (d, $^{4}J_{CF}$ = 3.0 Hz, C-1'), 129.2 (d, $^{3}J_{CF}$ = 8.9 Hz, C-2' and C-6'), 161.3 (d, $^{1}J_{CF}$ = 245.0 Hz, C-1'), 176.8 (2 x C=O).

***N*-(4-chlorophenyl)succinimide (4e)**

White solid; yield: 210 mg (50%); mp 163-165 °C (MeOH), lit.[3] 170 °C.

^{1}H NMR (300 MHz, DMSO-d_6): δ 2.78 (4H, s, CH_2CH_2), 7.31 (2H, d, ^{3}J = 8.8 Hz, H-2' and H-6'), 7.56 (2H, d, ^{3}J = 8.9 Hz, H-3' and H-5').

^{13}C NMR (75 MHz, DMSO-d_6): δ 28.4 (CH_2CH_2), 128.7 (C-2' and C-6'), 128.8 (C-3' and C-5'), 131.5 (C-1'), 132.5 (C-4'), 176.6 (2 x C=O).

***N*-(4-methylphenyl)succinimide (4g)**

White solid; yield: 127 mg (34%); mp 151-152 °C (THF), lit.[3] 154-155 °C.

^{1}H NMR (300 MHz, DMSO-d_6): δ 2.34 (3H, s, CH_3), 2.76 (4H, s, CH_2CH_2), 7.12 (2H, d, ^{3}J = 8.4 Hz, H-2' and H-6'), 7.28 (2H, d, ^{3}J = 8.3 Hz, H-3' and H-5').

^{13}C NMR (75 MHz, DMSO-d_6): δ 20.6 (CH_3), 28.3 (CH_2CH_2), 126.8 (C-2' and C-6'), 129.2 (C-3' and C-5'), 130.0 (C-1'), 137.5 (C-4'), 176.9 (2 x C=O).

***N*-(4-methoxyphenyl)succinimide (4j)**

Purple solid; yield: 328 mg (80%); mp 163-165 °C (MeOH), lit.[4] 165-167 °C.

^{1}H NMR (300 MHz, DMSO-d_6): δ 2.75 (4H, s, CH_2CH_2), 3.77 (3H, s, OCH_3), 7.02 (2H, d, ^{3}J = 9.1 Hz, H-2' and H-6'), 7.16 (2H, d, ^{3}J = 9.1 Hz, H-3' and H-5').

^{13}C NMR (75 MHz, DMSO-d_6): δ 28.3 (CH_2CH_2), 55.2 (OCH_3), 114.0 (C-3' and C-5'), 125.2 (C-1'), 128.2 (C-2' and C-6'), 158.7 (C-4'), 177.0 (2 x C=O).

***N*-(4-(*N'*-acetamido)phenyl)succinimide (4k)**

Brown solid; yield: 446 mg (96%); mp 254-255 °C (MeOH).

^{1}H NMR (300 MHz, DMSO-d_6): δ 2.06 (3H, s, CH_3), 2.76 (4H, s, CH_2CH_2), 7.17 (2H, d, ^{3}J = 8.4 Hz, H-2' and H-6'), 7.66 (2H, d, ^{3}J = 8.6 Hz, H-3' and H-5'), 10.07 (1H, br s, NH).

^{13}C NMR (75 MHz, DMSO-d_6): δ 23.9 (CH_3), 28.3 (CH_2CH_2), 119.0 (C-3' and C-5'), 127.3 (C-1', C-2' and C-6'), 138.9 (C-4'), 168.4 (C=O), 176.9 (2 x C=O).

Synthesis of *N*-(4-isopropylphenyl)succinimide (4h)

A mixture of 4-isopropylyaniline (1.37 g, 10 mmol), succinic anhydride (1.50 g, 15 mmol) and N,N-diisopropylethylamine (348 µL, 2 mmol) in tetrahydrofuran (10 mL) was irradiated in 30 mL seamless pressure vial using microwave system operating at maximal microwave power up to 300 W at 180 °C for 15 min. After cooling, the solvent was evaporated under vacuum. The resultant residue was mixed with aqueous solution of sodium bicarbonate (1.2 M, 10 mL) and stirred for 10 min at room temperature. The precipitate was filtered and washed with cold water. Analytical sample was recrystallised from aqueous methanol.

White solid; yield: 1.5 g (70%); mp 127-129 °C (MeOH/H_2O).

^{1}H NMR (300 MHz, DMSO-d_6): δ 1.22 (6H, d, ^3J = 6.9 Hz, CH_3CH_3), 2.77 (4H, s, CH_2CH_2), 2.93 (1H, m, ^3J = 6.9 Hz, CH), 7.16 (2H, d, ^3J = 8.4 Hz, H-2' and H-6'), 7.34 (2H, d, ^3J = 8.3 Hz, H-3' and H-5').

^{13}C NMR (75 MHz, DMSO-d_6): δ 23.7 (CH_3CH_3), 28.3 (CH_2CH_2), 33.1 (CH), 126.6 (C-3' and C-5'), 126.9 (C-2' and C-6'), 130.3 (C-1'), 148.3 (C-4'), 176.9 (2 x C=O).

***N*-Arylsuccinamic acids 6; General Procedure**

A mixture of arylamine (20 mmol) and succinic anhydride (2.40 g, 24 mmol) were heated under reflux in 25 mL of toluene for 2.5 h. After cooling, the precipitate was filtered and washed with toluene and hexane. Analytical sample was recrystallised from toluene.

***N*-(2-chlorophenyl)succinamic acid (6a)**

White solid; yield: 4.49 g (99%); mp 145-146 °C (PhMe), lit.[5] 145-148 °C.

^{1}H NMR (300 MHz, DMSO-d_6): δ 2.51-2.53 (2H, m, CH_2CONH), 2.61-2.65 (2H, br t, CH_2COOH), 7.17 (1H, dt, ^4J = 1.8 Hz, ^3J = 7.7 Hz, H-4'), 7.31 (1H, dt, ^4J = 1.4 Hz, ^3J = 7.7 Hz, H-5'), 7.47 (1H, dd, ^4J = 1.5 Hz, ^3J = 8.0 Hz, H-6'), 7.71 (1H, dd, ^4J = 1.4 Hz, ^3J = 8.1 Hz, H-3').

^{13}C NMR (75 MHz, DMSO-d_6): δ 28.9 (CH_2), 30.5 (CH_2), 125.9-126.1 (C-2', C-4' and C-6'), 127.2 (C-5'), 129.3 (C-3'), 134.9 (C-1'), 170.4 (NHCO), 173.6 (COOH).

***N*-(3-chlorophenyl)succinamic acid (6b)**

White powder; yield: 4.05 g (89%); mp 111-113 °C (PhMe).

^{1}H NMR (300 MHz, DMSO-d_6): δ 2.54-2.51 (4H, m, CH_2CH_2), 7.07 (1H, ddd, ^4J = 1.0 Hz, ^4J = 2.1 Hz, ^3J = 7.9 Hz, H-4'), 7.31 (1H, t, ^3J = 8.1 Hz, H-5'), 7.42 (1H, ddd, ^4J '= 1.1 Hz, ^4J = 1.9 Hz, ^3J = 8.2 Hz, H-6'), 7.80 (1H, dd, ^4J = 2.0 Hz, ^4J = 2.0 Hz, H-2').

^{13}C NMR (75 MHz, DMSO-d_6): δ 28.6 (CH_2), 31.0 (CH_2), 117.1 (C-6'), 118.3 (C-2'), 122.5 (C-4'), 130.3 (C-5'), 132.9 (C-3'), 140.6 (C-1'), 170.4 (NHCO), 173.7 (COOH).

***N*-(3-methylphenyl)succinamic acid (6c)**

White solid; yield: 4.14 g (99%); mp 134-136 °C (PhMe), lit.[5] 136-140 °C.

^{1}H NMR (300 MHz, DMSO-d_6): δ 2.26 (3H, s, CH_3), 2.49-2.57 (4H, m, CH_2CH_2), 6.83 (1H, d, ^3J = 7.5 Hz, H-4'), 7.15 (1H, t, ^3J = 7.8 Hz, H-5'), 7.35 (1H, d, ^3J = 7.4 Hz, H-6'), 7.43 (1H, s, H-2').

^{13}C NMR (75 MHz, DMSO-d_6): δ 21.1 (CH_3), 28.7 (CH_2), 30.9 (CH_2), 116.0 (C-6'), 119.4 (C-2'), 123.5 (C-4'), 128.4 (C-5'), 137.7 (C-3'), 139.1 (C-1'), 169.9 (NHCO), 173.7 (COOH).

***N*-(3-methoxyphenyl)succinamic acid (6d)**

White solid; yield: 3.48 g (78%); mp 106-107 °C (PhMe).

^{1}H NMR (300 MHz, DMSO-d_6): δ 2.48-2.58 (4H, m, CH_2CH_2), 3.72 (3H, s, OCH_3), 6.60 (1H, ddd, ^4J = 1.0 Hz, ^4J = 2.5 Hz, ^3J = 8.1 Hz, H-4'), 7.10 (1H, ddd, ^4J = 1.1 Hz, ^4J = 1.6 Hz, ^3J = 8.1 Hz, H-6'), 7.18 (1H, t, ^3J = 8.0 Hz, H-5'), 7.31 (1H, dd, ^4J = 2.1 Hz, ^4J = 2.1 Hz, H-2').

^{13}C NMR (75 MHz, DMSO-d_6): δ 28.7 (CH_2), 31.0 (CH_2), 104.6 (C-2'), 108.3 (C-4'), 111.1 (C-6'), 129.3 (C-5'), 140.4 (C-1'), 159.4 (C-3'), 170.0 (NHCO), 173.7 (COOH).

***N*-Arylsuccinimides 4c, 4d, 4f, and 4i; General Procedure**

A mixture of *N*-arylsuccinamic acid (**6**) (20 mmol) and potassium acetate (5.89 g, 60 mmol) in acetic anhydride (66.70 mL) was heated under reflux for 1 h. After cooling, the solvent was evaporated under vacuum. To the resultant reaction mixture was added aqueous sodium carbonate (0.8 M, 50 mL), stirred for 10 min at room temperature and extracted using dichloromethane (3 x 20 ml). The organic layer was collected and dried over magnesium sulphate overnight and evaporated under vacuum. The crude product was washed with diethyl ether and filtered. Analytical sample was recrystallised from a suitable solvent.

***N*-(2-chlorophenyl)succinimide (4c)**

Light brown solid; yield: 3.52 g (84%); mp 110-112 °C (Et_2O).

^{1}H NMR (300 MHz, DMSO-d_6): δ 2.78 (4H, s, CH_2CH_2), 7.24-7.27 (2H, m, H-2' and H-6'), 7.38-7.43 (1H, m, H-4'), 7.45-7.51 (2H, m, H-3' and H-5').

^{13}C NMR (75 MHz, DMSO-d_6): δ 28.5 (CH_2CH_2), 128.0 (C-1'), 129.7 (C-5'), 130.5 (C-3' and C-6'), 130.7 (C-4'), 131.3 (C-2'), 176.0 (2 x C=O).

***N*-(3-chlorophenyl)succinimide (4d)**

White solid; yield: 3.73 g (89%); mp 117-119 °C (H_2O), lit.[2] 107-109 °C.

^{1}H NMR (300 MHz, DMSO-d_6): δ 2.78 (4H, s, CH_2CH_2), 7.27 (1H, ddd, ^4J = 1.8 Hz, ^4J = 1.8 Hz, ^3J = 7.2 Hz, H-6'), 7.39-7.40 (1H, m, H-2'), 7.46-7.50 (2H, m, H-4' and H-5').

^{13}C NMR (75 MHz, DMSO-d_6): δ 28.4 (CH_2CH_2), 125.8 (C-6'), 126.9 (C-2'), 128.0 (C-4'), 130.3 (C-5'), 132.8 (C-3'), 134.0 (C-1'), 176.5 (2 x C=O).

***N*-(3-methylphenyl)succinimide (4f)**

Brown solid; yield: 3.46 g (92%); mp 112-114 °C (H_2O), lit.[4] 103-105 °C.

^{1}H NMR (300 MHz, DMSO-d_6): δ 2.33 (3H, s, CH_3), 2.77 (4H, s, CH_2CH_2), 7.03-7.06 (2H, m, H-2' and H-6'), 7.22 (1H, d, ^3J = 7.6 Hz, H-4'), 7.36 (1H, t, ^3J = 7.7 Hz, H-5').

^{13}C NMR (75 MHz, DMSO-d_6): δ 20.7 (CH_3), 28.4 (CH_2CH_2), 124.1 (C-6'), 127.4 (C-2'), 128.5 (C-5'), 128.7 (C-4'), 132.6 (C-1'), 138.1 (C-3'), 176.8 (2 x C=O).

***N*-(3-methoxyphenyl)succinimide (4i)**

Light brown solid; yield: 2.91 g (71%); mp 80-82 °C (Et_2O).

^{1}H NMR (300 MHz, DMSO-d_6): δ 2.77 (4H, s, CH_2CH_2), 3.76 (3H, s, OCH_3), 6.81-6.84 (2H, m, H-2' and H-6'), 7.00 (1H, ddd, ^4J = 1.0 Hz, ^4J = 2.5 Hz, ^3J = 8.4 Hz,' H-4'), 7.39 (1H, t, ^3J = 8.3 Hz, H-5')

^{13}C NMR (75 MHz, DMSO-d_6): δ 28.4 (CH_2CH_2), 55.2 (OCH_3), 112.9 (C-2'), 113.6 (C-4'), 119.3 (C-6'), 129.5 (C-5'), 133.8 (C-1'), 159.3 (C-3'), 176.7 (2 x C=O).

References

1. Chernyshev, V. M.; Chernysheva, A. V.; Starikova, Z. A. *Heterocycles* **2010,** *81*, 2291.
2. Garad, D. N.; Tanpure, S. D.; Mhaske, S. B. *Beilstein J. Org. Chem.* **2015,** *11,* 1008.
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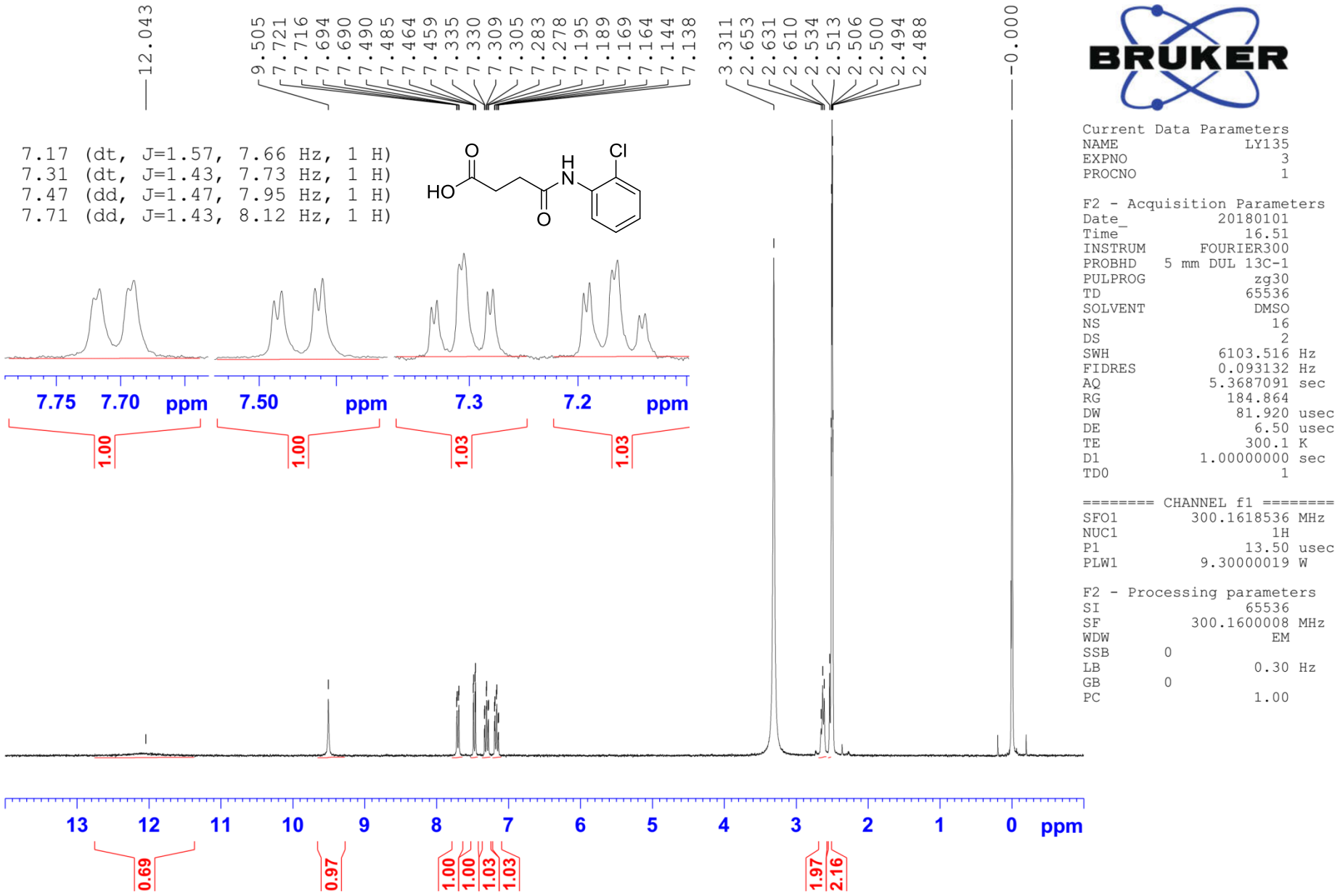
5. Habash, M.; Taha, M. O. *Bioorg. Med. Chem.* **2011,** *19*, 4746.

^{1}H and ^{13}C NMR spectra of succinamic acids 6

N-(2-chlorophenyl)succinamic acid (6a)

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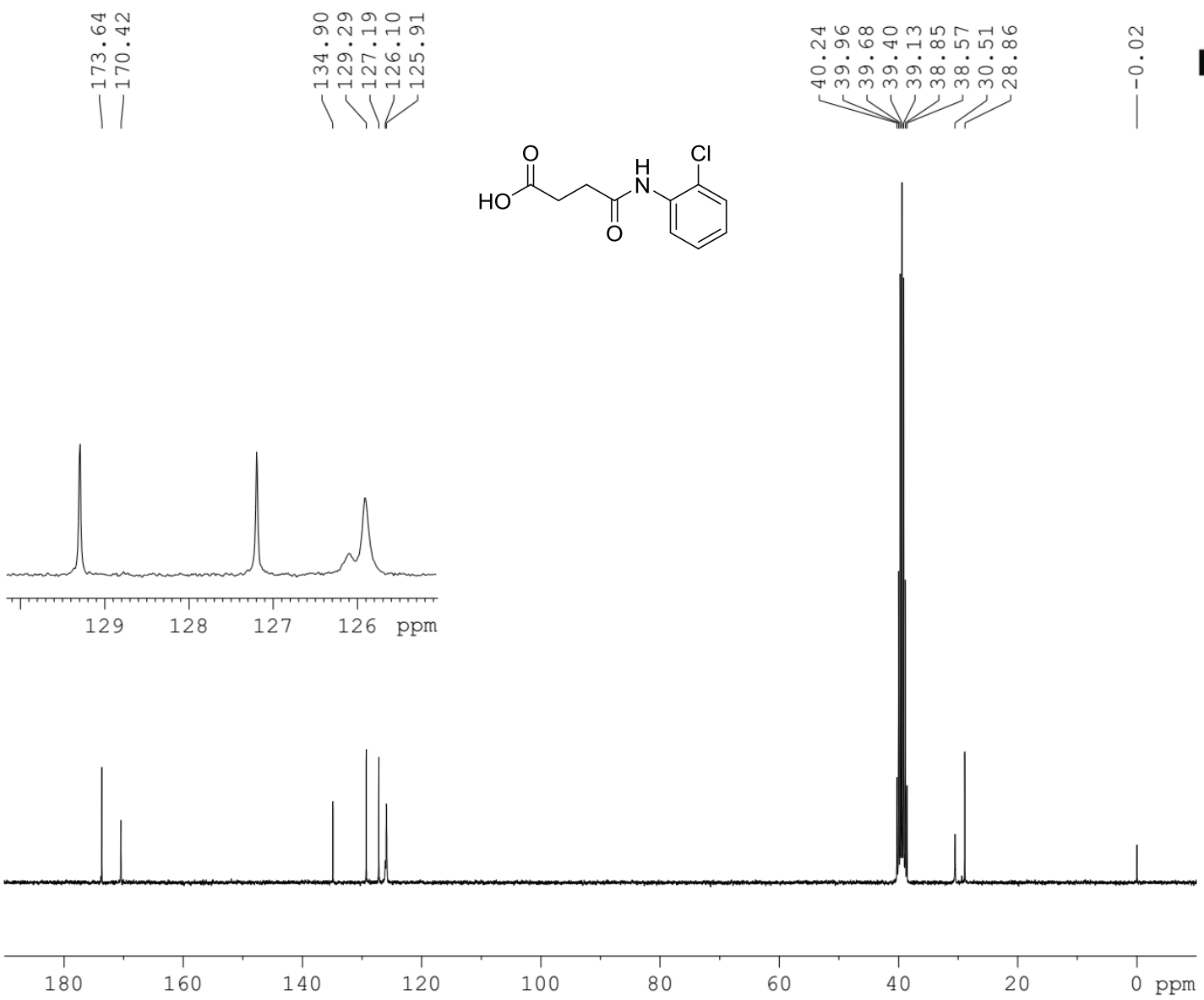
N-(2-chlorophenyl)succinamic acid (6a)

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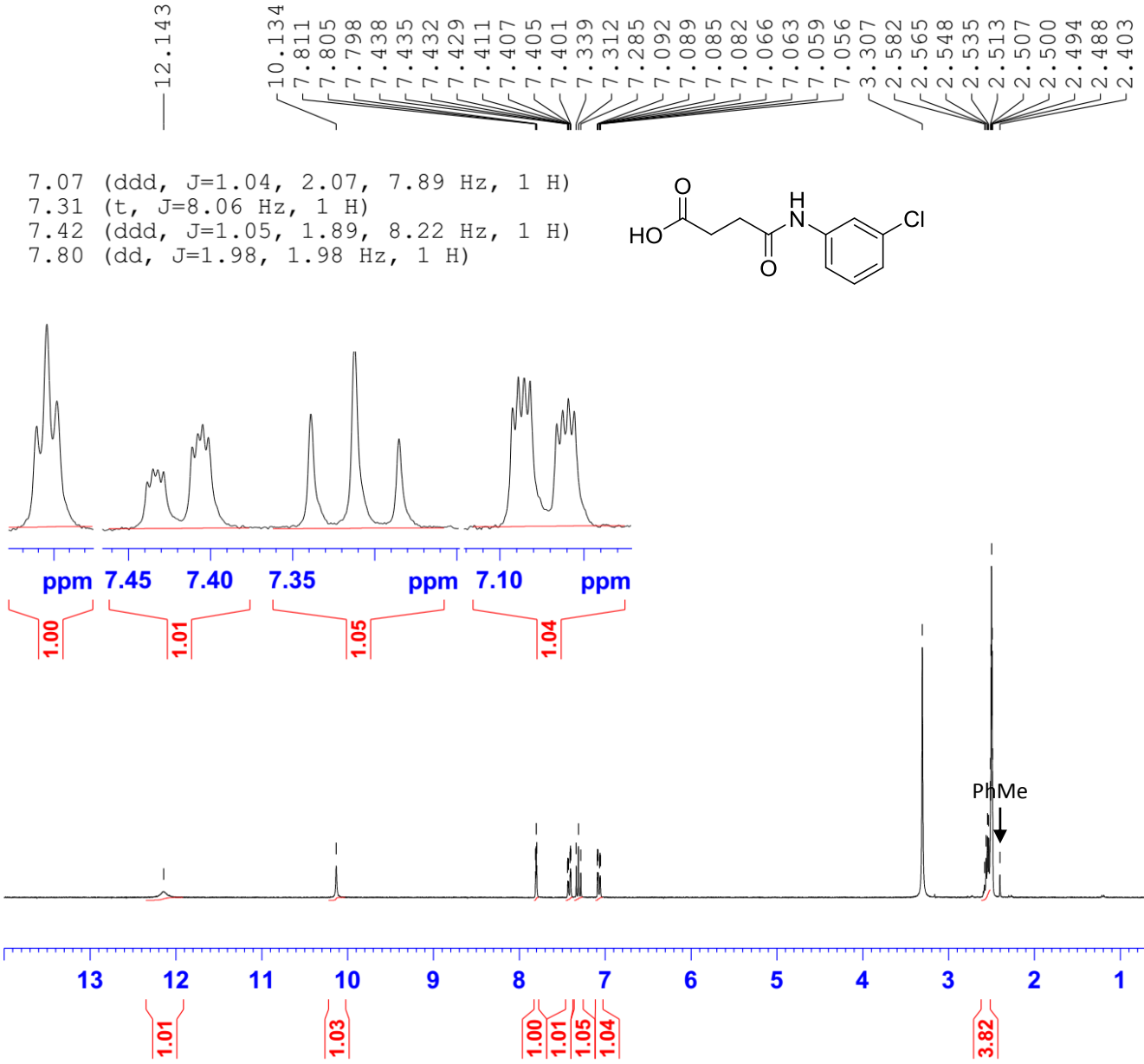


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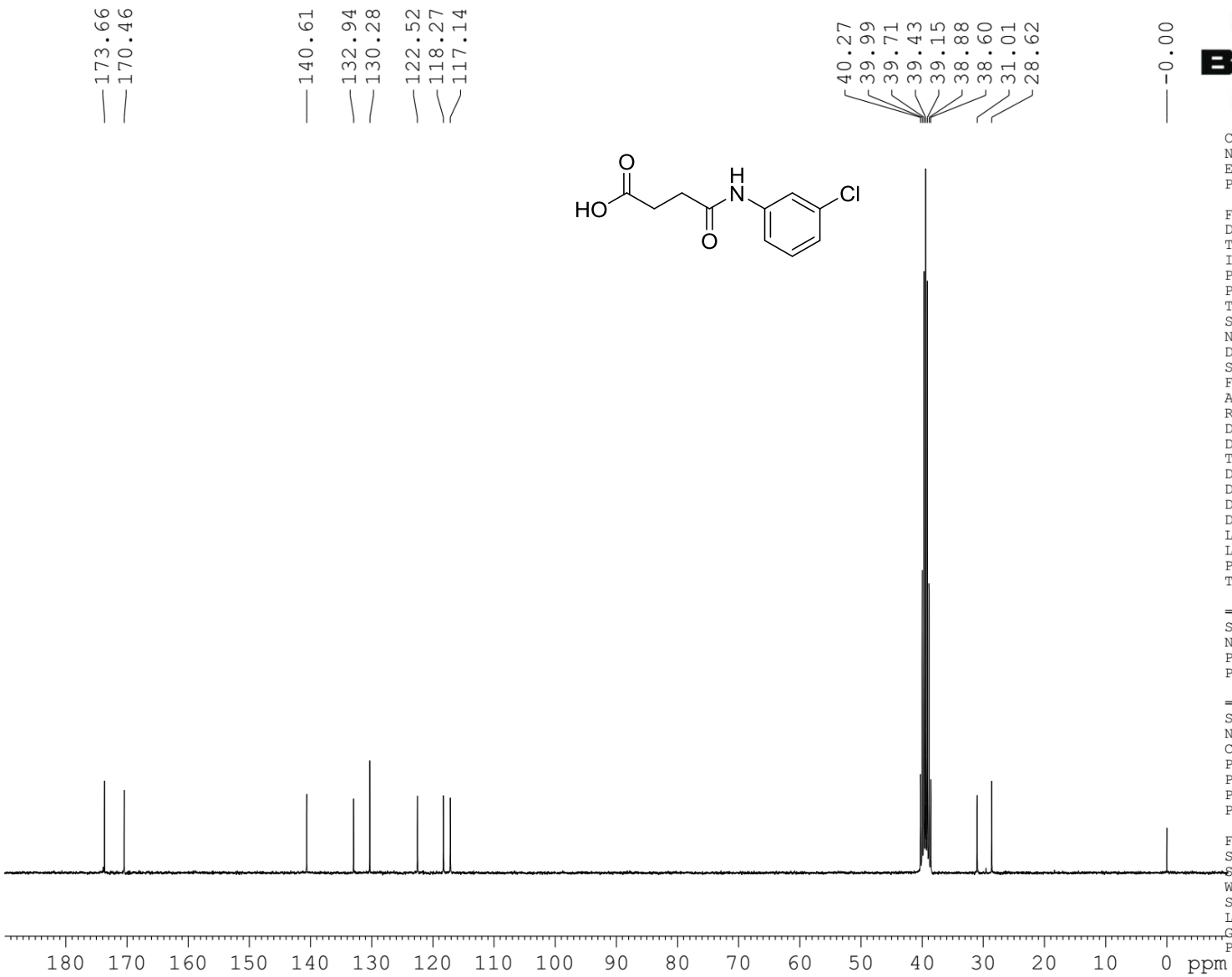
N-(3-chlorophenyl)succinamic acid (6b)



BRUKER

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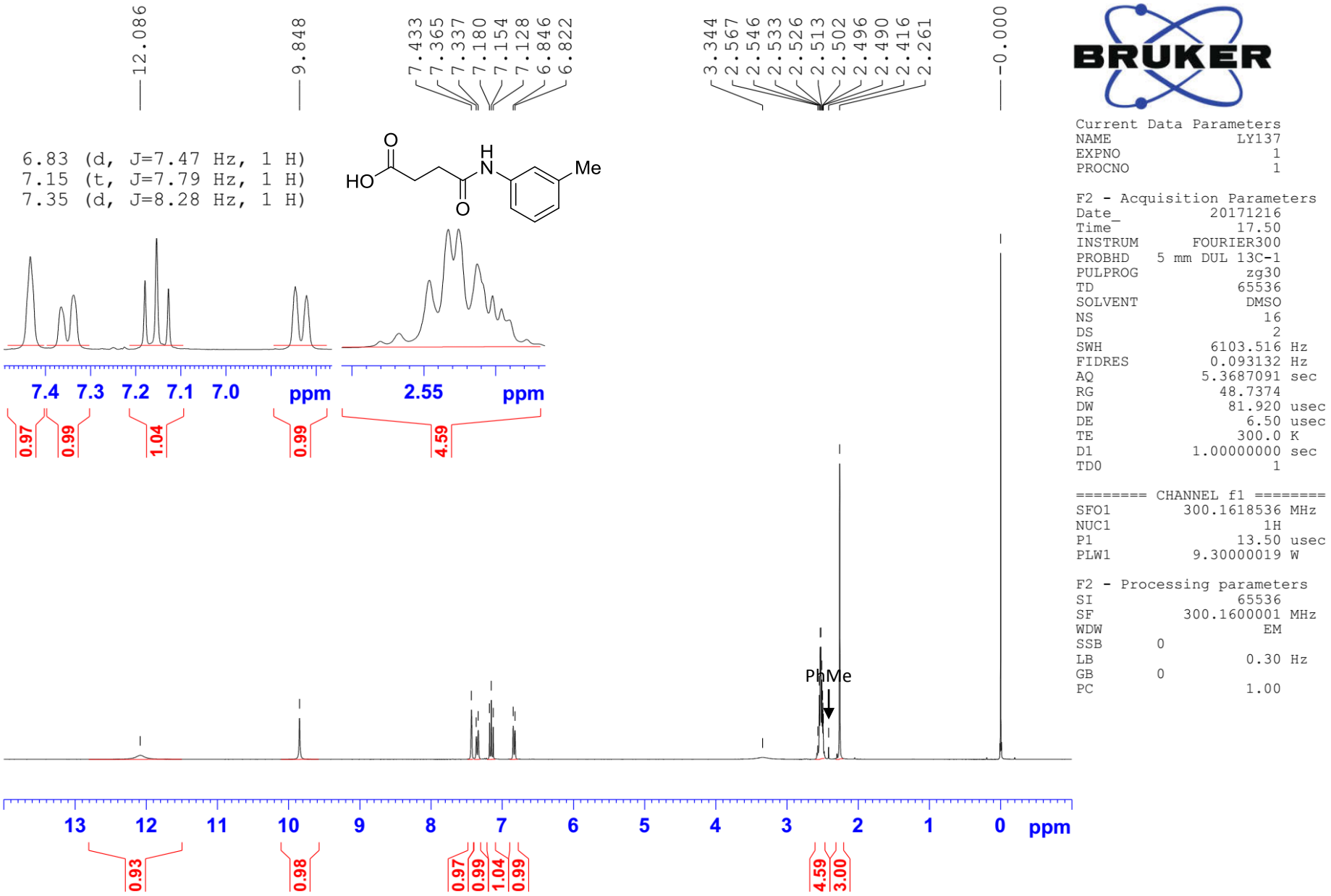
N-(3-methylphenyl)succinamic acid (6c)

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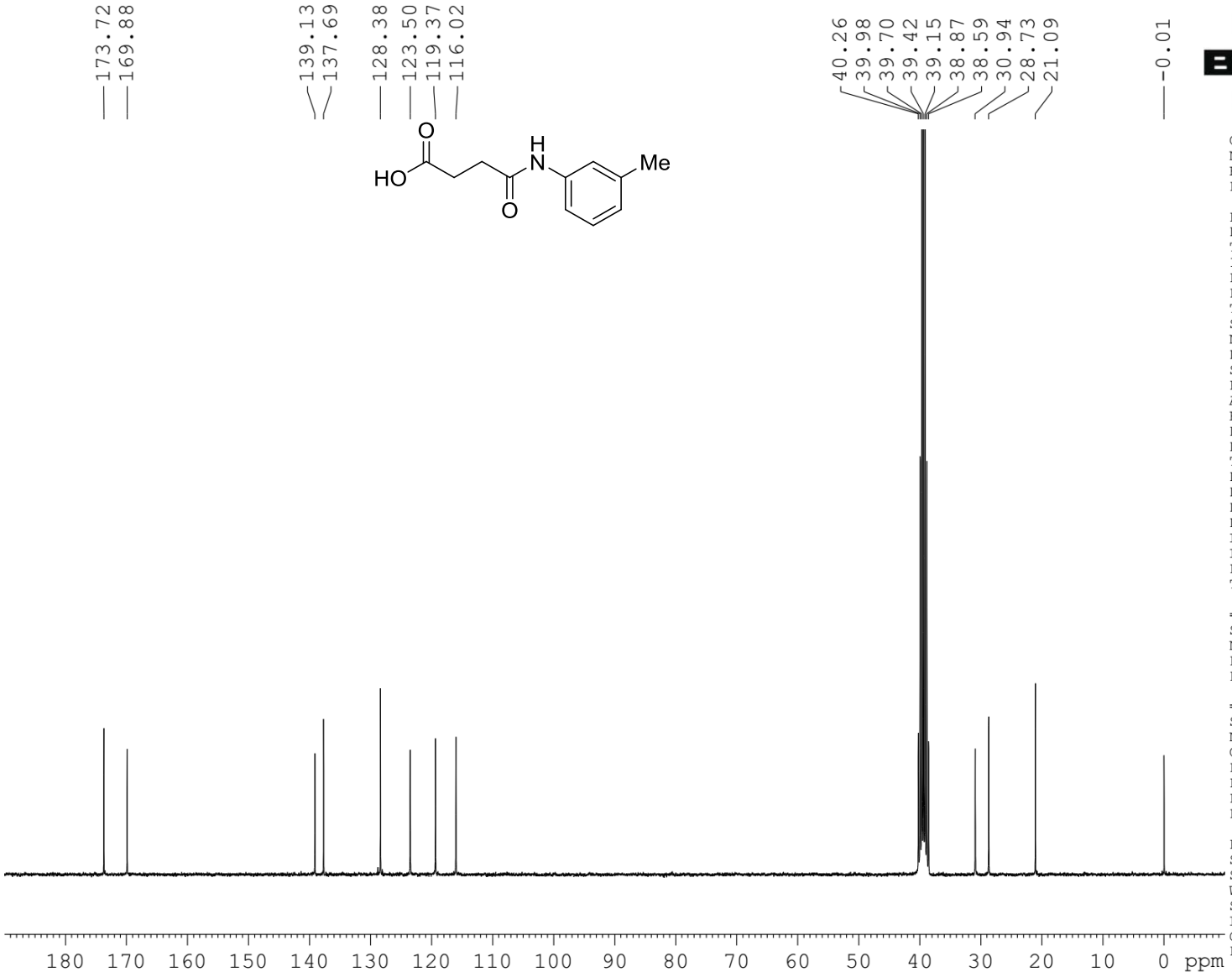
N-(3-methylphenyl)succinamic acid (6c)



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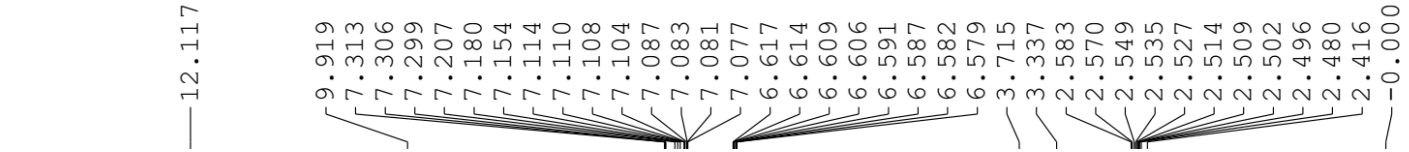
AQ                 1.3421773 sec
RG                   501.187
DW                    20.480 usec
DE                     6.50 usec
TE                    300.1 K
D1                 2.00000000 sec
D11                0.03000000 sec
D31                0.00001500 sec
D40                0.00439029 sec
L4                        37
L5                        53
P32                   98.00 usec
TD0                       7

======== CHANNEL f1 ========
SFO1              75.4828392 MHz
NUC1                     13C
P1                    15.00 usec
PLW1             22.00000000 W

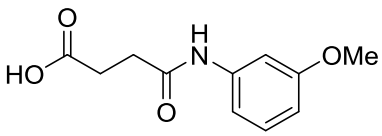
======== CHANNEL f2 ========
SFO2             300.1612006 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                 98.00 usec
PLW2              9.30000019 W
PLW12             0.29359001 W
PLW13             0.20359001 W

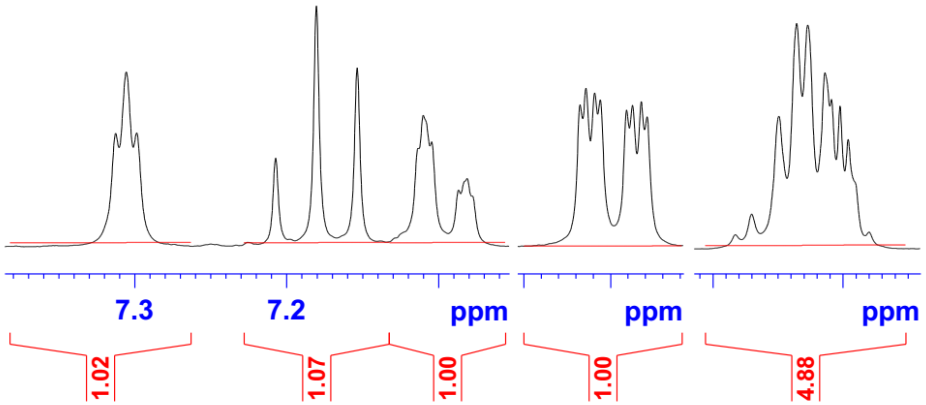
F2 - Processing parameters
SI                       32768
SF                75.4753342 MHz
WDW                         EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

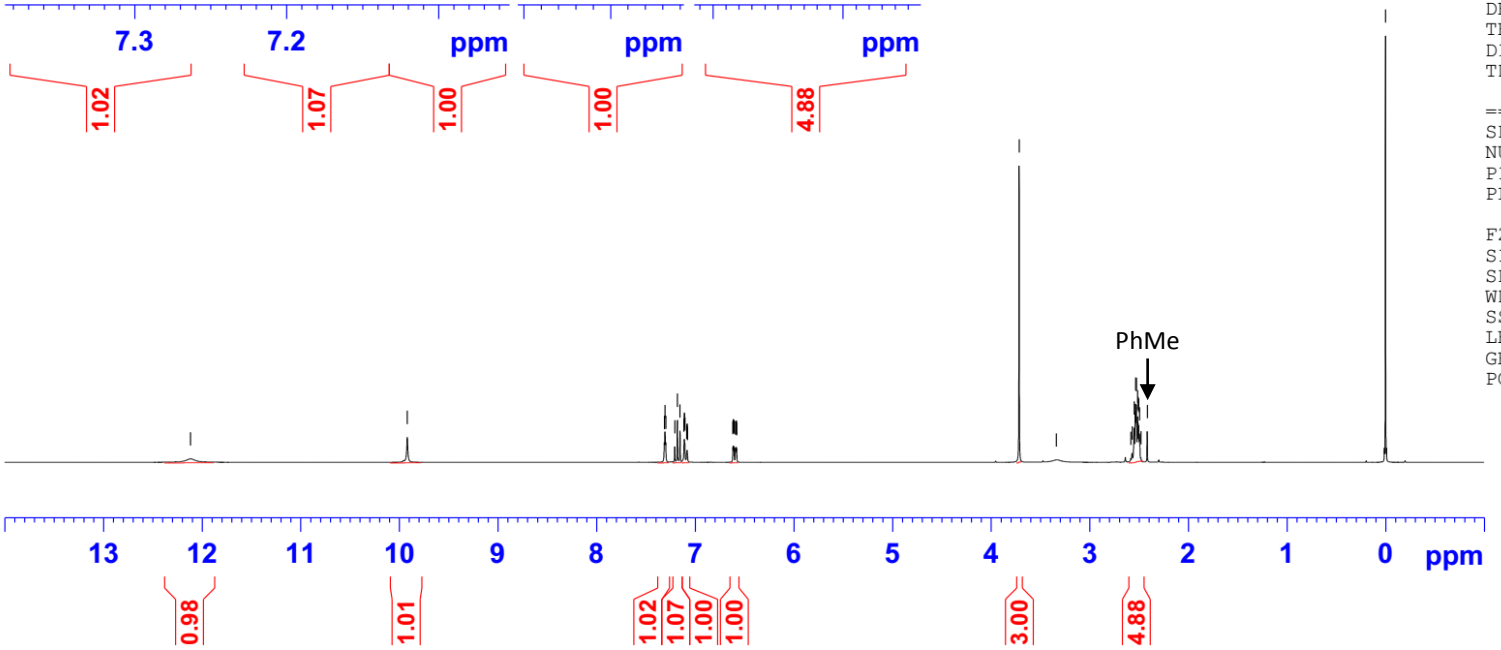
N-(3-methoxyphenyl)succinamic acid (6d)



6.60 (ddd, J=1.01, 2.51, 8.06 Hz, 1 H)
7.10 (ddd, J=1.10, 1.64, 8.08 Hz, 1 H)
7.18 (t, J=8.04 Hz, 1 H)
7.31 (dd, J=2.09, 2.09 Hz, 1 H)







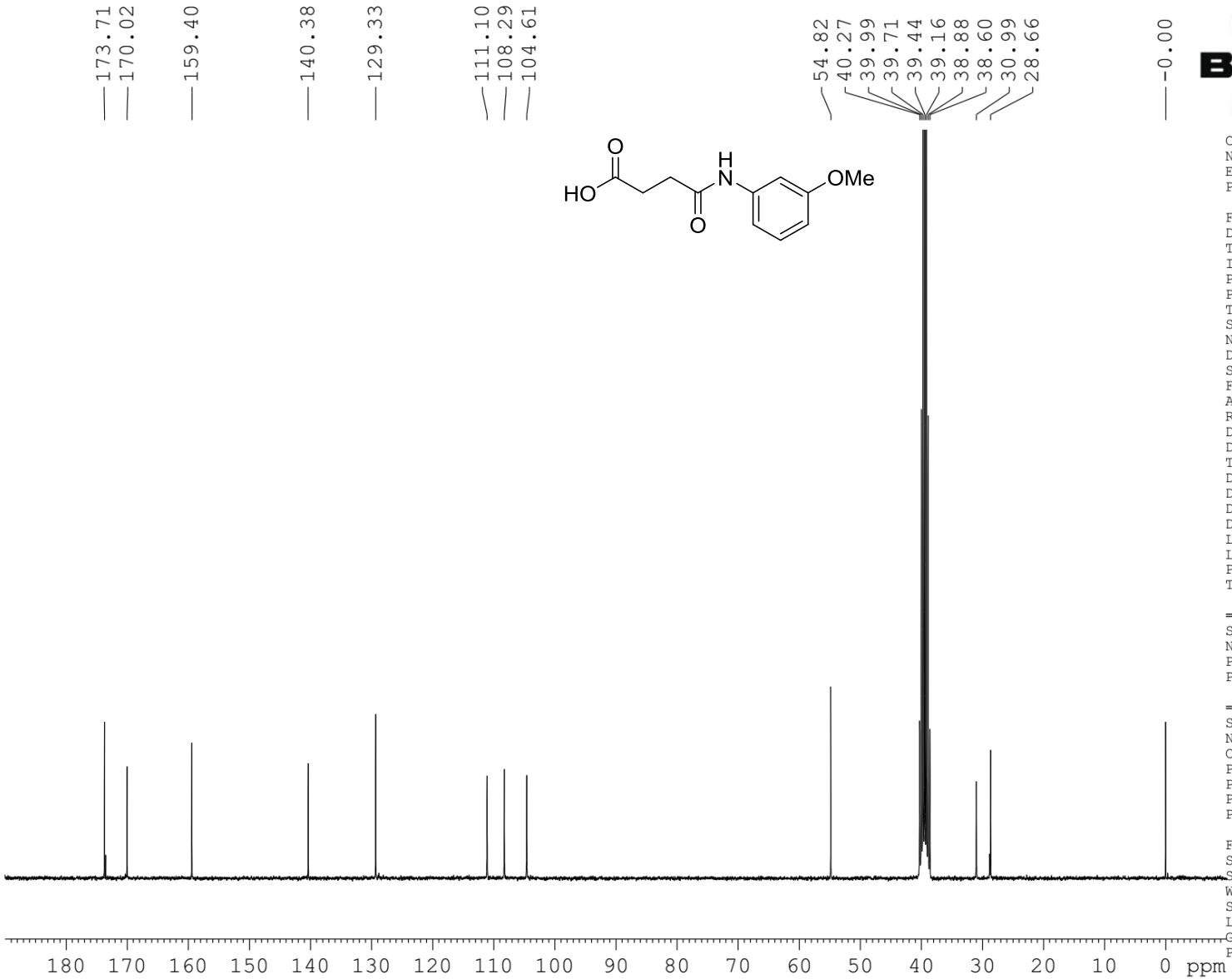

```
Current Data Parameters
NAME                  LY138
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20171216
Time                  17.54
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT               DMSO
NS                      16
DS                       2
SWH               6103.516 Hz
FIDRES           0.093132 Hz
AQ               5.3687091 sec
RG                  76.8407
DW                  81.920 usec
DE                    6.50 usec
TE                   300.0 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1          300.1618536 MHz
NUC1                     1H
P1                    13.50 usec
PLW1           9.30000019 W

F2 - Processing parameters
SI                    65536
SF            300.1600001 MHz
WDW                      EM
SSB         0
LB                    0.30 Hz
GB          0
PC                    1.00
```

N-(3-methoxyphenyl)succinamic acid (6d)



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```
Current Data Parameters
NAME                  LY138
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20171219
Time                   0.04
INSTRUM          FOURIER300
PROBHD     5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                     7168
DS                        4
SWH               24414.063 Hz
FIDRES             0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                   20.480 usec
DE                    6.50 usec
TE                   300.1 K
D1              2.00000000 sec
D11             0.03000000 sec
D31             0.00001500 sec
D40             0.00439029 sec
L4                       37
L5                       53
P32                   98.00 usec
TD0                       7

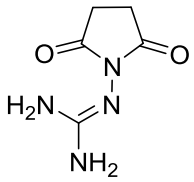
======== CHANNEL f1 ========
SFO1            75.4828392 MHz
NUC1                    13C
P1                    15.00 usec
PLW1           22.00000000 W

======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                    1H
CPDPRG[2            waltz16
PCPD2                 98.00 usec
PLW2            9.30000019 W
PLW12           0.29359001 W
PLW13           0.20359001 W

F2 - Processing parameters
SI                     32768
SF              75.4753341 MHz
WDW                       EM
SSB         0
LB                     1.00 Hz
GB          0
PC                     1.40
```

^{1}H and ^{13}C NMR spectra of succimimides 2 and 4

***N*-guanidinosuccinimide (2)**



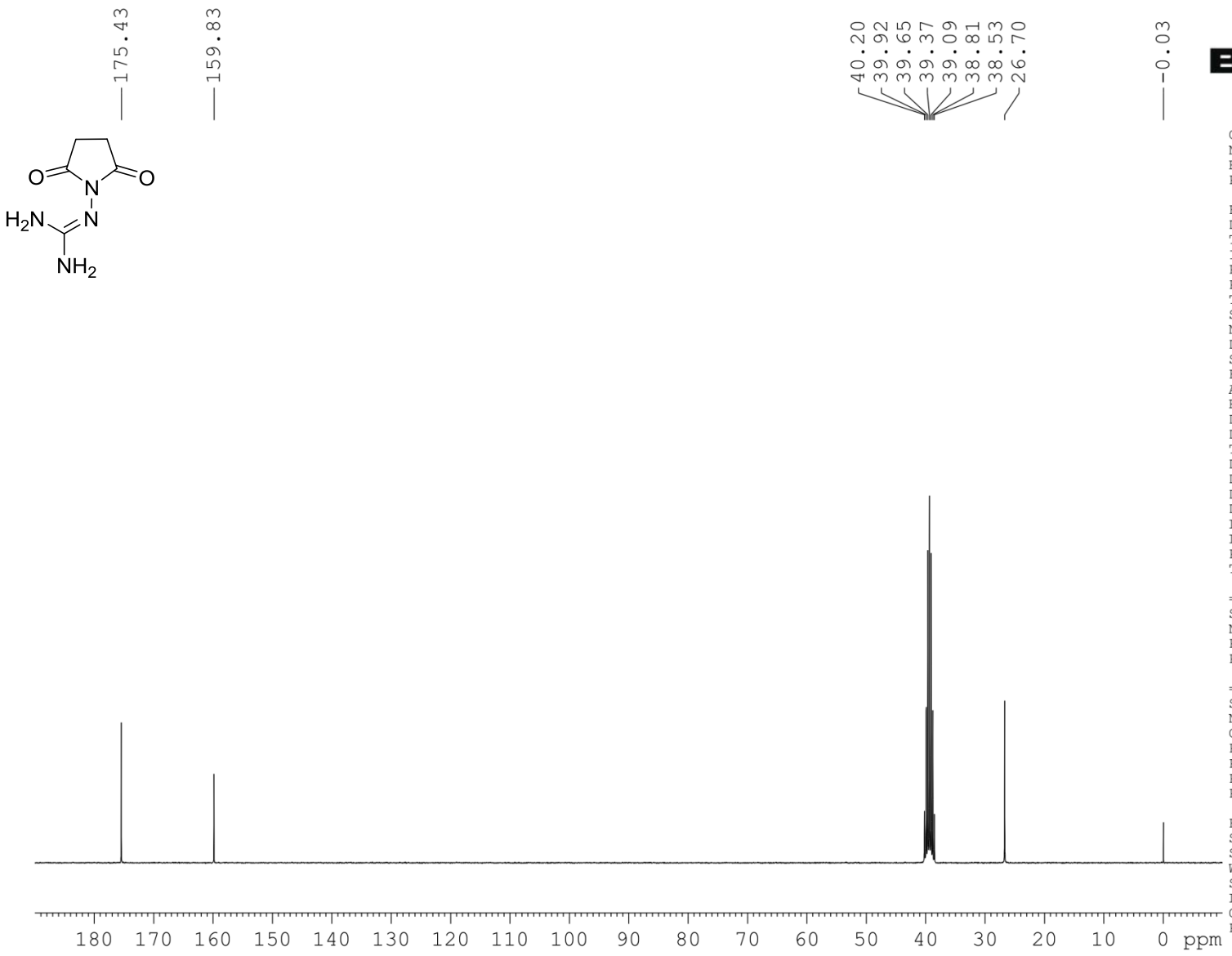

```
Current Data Parameters
NAME                  LY143
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20171226
Time                  15.45
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       16
DS                        2
SWH                6103.516 Hz
FIDRES            0.093132 Hz
AQ                5.3687091 sec
RG                  48.7008
DW                  81.920 usec
DE                    6.50 usec
TE                   300.0 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           300.1618536 MHz
NUC1                     1H
P1                    13.50 usec
PLW1           9.30000019 W

F2 - Processing parameters
SI                    65536
SF             300.1600001 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

N-guanidinosuccinimide (2)



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```
Current Data Parameters
NAME                  LY143
EXPNO                     2
PROCNO                    1

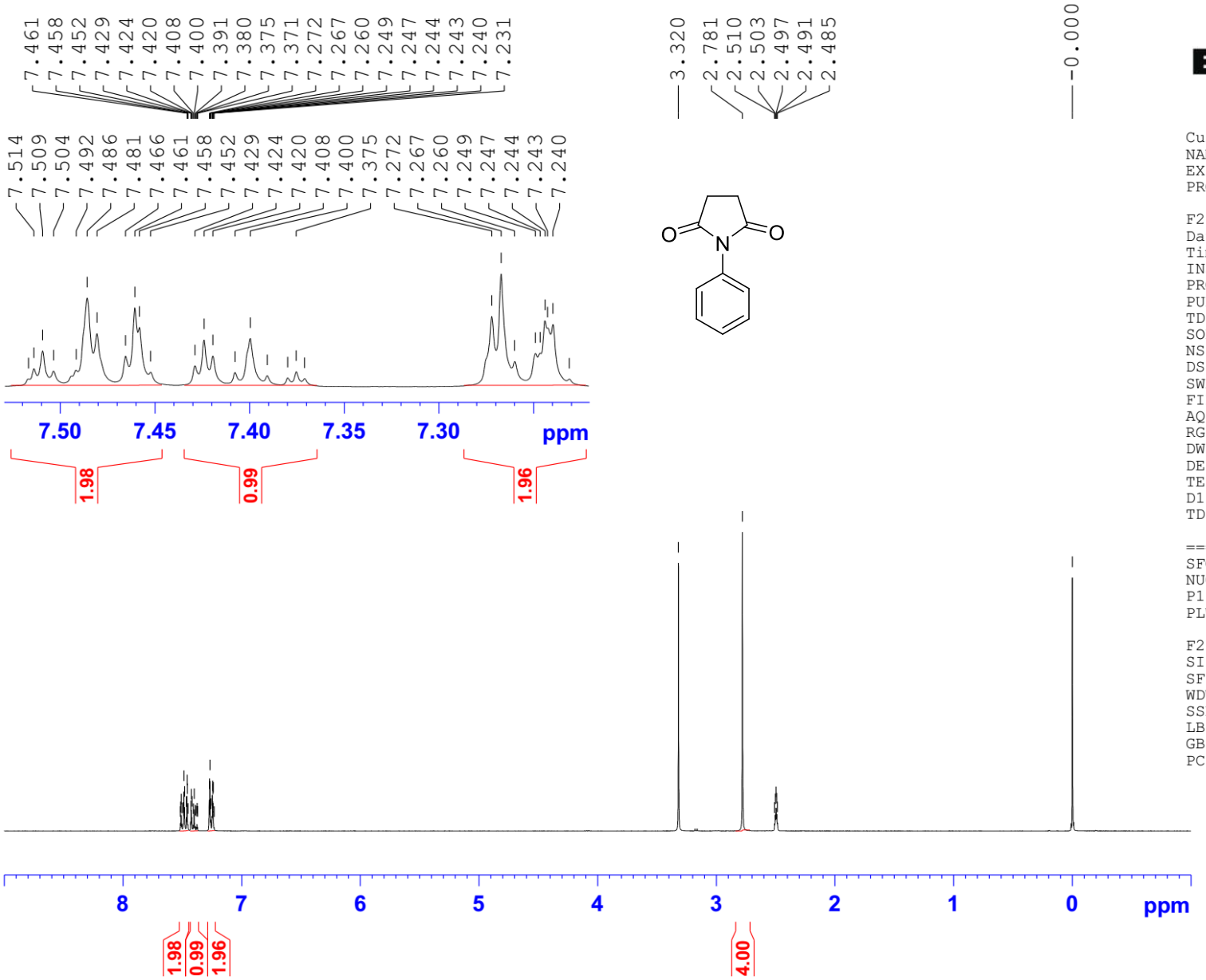
F2 - Acquisition Parameters
Date_              20171230
Time                 21.23
INSTRUM          FOURIER300
PROBHD     5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                    8192
DS                       4
SWH              24414.063 Hz
FIDRES               0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                   20.480 usec
DE                    6.50 usec
TE                   300.1 K
D1              2.00000000 sec
D11             0.03000000 sec
D31             0.00001500 sec
D40             0.00439029 sec
L4                       37
L5                       53
P32                  98.00 usec
TD0                      8

======== CHANNEL f1 ========
SFO1            75.4828392 MHz
NUC1                   13C
P1                   15.00 usec
PLW1          22.00000000 W

======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2                98.00 usec
PLW2            9.30000019 W
PLW12           0.29359001 W
PLW13           0.20359001 W

F2 - Processing parameters
SI                   32768
SF              75.4753376 MHz
WDW                     EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

N-phenylsuccinimide (4a)



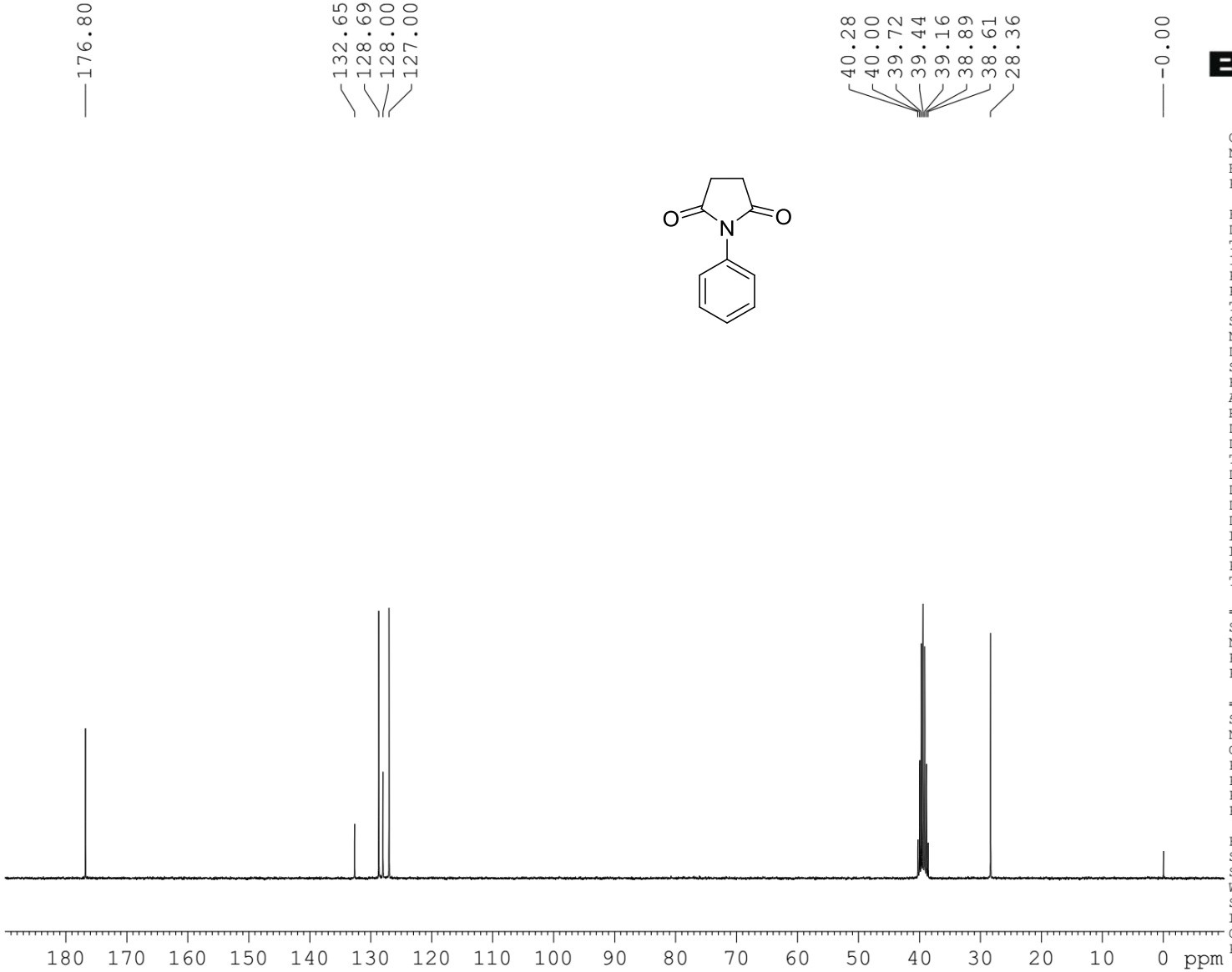

```
Current Data Parameters
NAME                  LY126
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20171226
Time                  15.27
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT               DMSO
NS                       16
DS                        2
SWH                6103.516 Hz
FIDRES            0.093132 Hz
AQ                5.3687091 sec
RG                   63.5979
DW                  81.920 usec
DE                   6.50 usec
TE                  300.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           300.1618536 MHz
NUC1                      1H
P1                   13.50 usec
PLW1            9.30000019 W

F2 - Processing parameters
SI                       65536
SF             300.1600017 MHz
WDW                        EM
SSB         0
LB                    0.30 Hz
GB          0
PC                    1.00
```

N-phenylsuccinimide (4a)




```
Current Data Parameters
NAME                  LY126
EXPNO                     2
PROCNO                    1

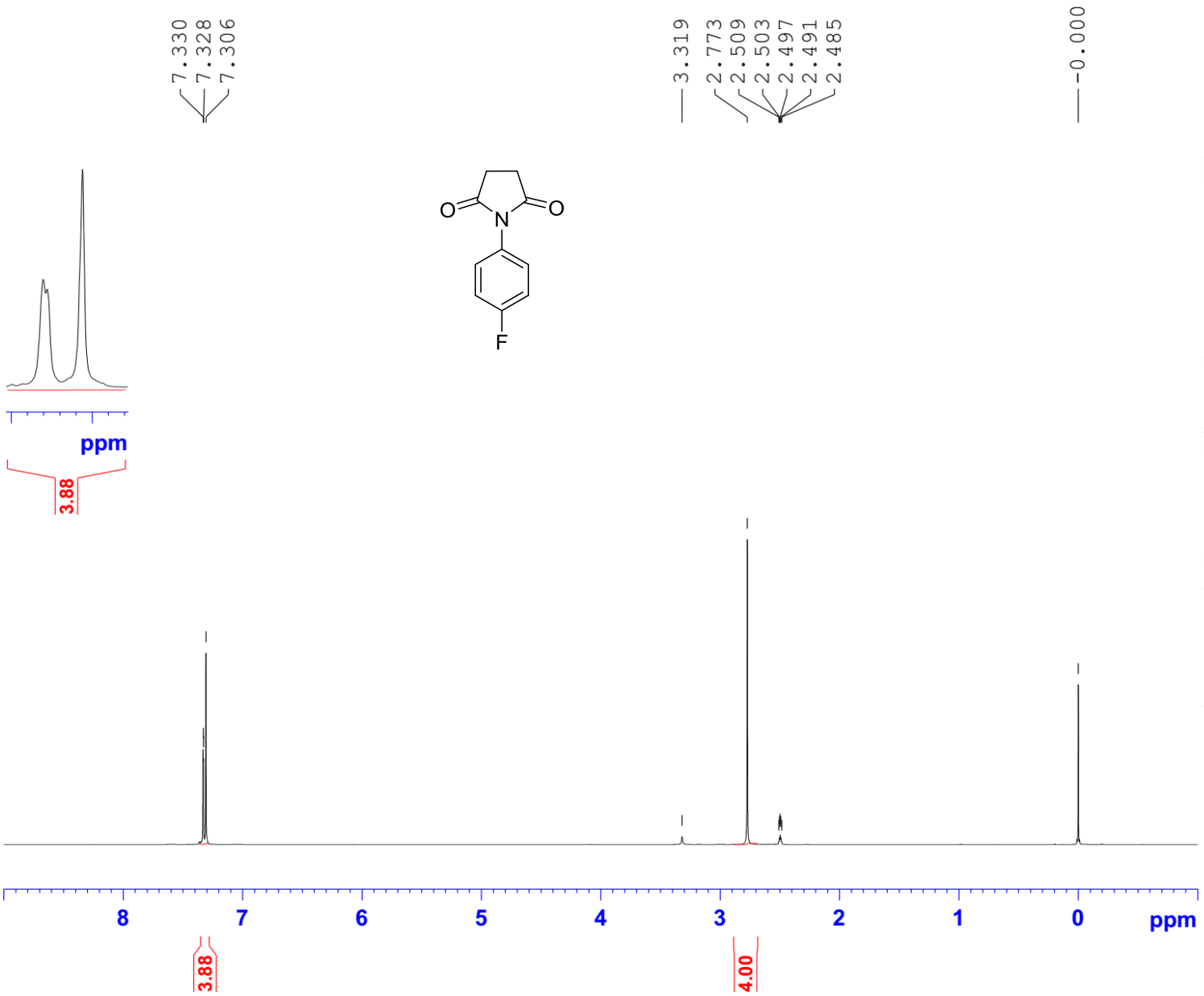
F2 - Acquisition Parameters
Date_              20171211
Time                  17.39
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                    65536
SOLVENT                DMSO
NS                     1024
DS                        4
SWH              24414.063 Hz
FIDRES            0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                   20.480 usec
DE                    6.50 usec
TE                   300.1 K
D1               2.00000000 sec
D11              0.03000000 sec
D31              0.00001500 sec
D40              0.00439029 sec
L4                       37
L5                       53
P32                   98.00 usec
TD0                       1

======== CHANNEL f1 ========
SFO1            75.4828392 MHz
NUC1                   13C
P1                    15.00 usec
PLW1           22.00000000 W

======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2                 98.00 usec
PLW2            9.30000019 W
PLW12           0.29359001 W
PLW13           0.20359001 W

F2 - Processing parameters
SI                    32768
SF              75.4753350 MHz
WDW                      EM
SSB         0
LB                    1.00 Hz
GB          0
PC                    1.40
```

N-(4-fluorophenyl)succinimide (4b)



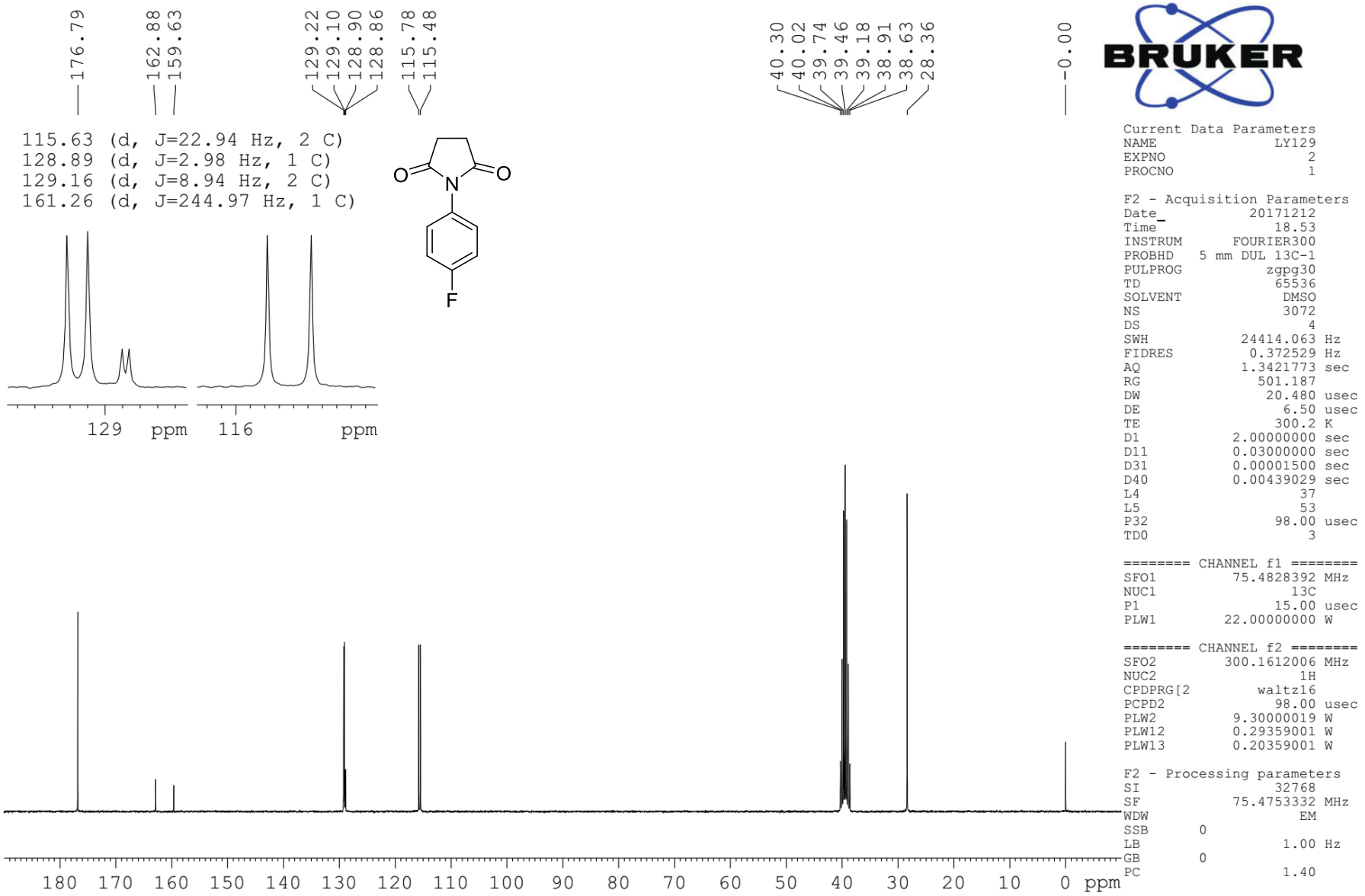

```
Current Data Parameters
NAME                  LY129
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20171212
Time                  17.53
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       16
DS                        2
SWH               6103.516 Hz
FIDRES            0.093132 Hz
AQ                5.3687091 sec
RG                   31.623
DW                   81.920 usec
DE                    6.50 usec
TE                   300.0 K
D1               1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           300.1618536 MHz
NUC1                     1H
P1                    13.50 usec
PLW1           9.30000019 W

F2 - Processing parameters
SI                    65536
SF             300.1600016 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

N-(4-fluorophenyl)succinimide (4b)




```
Current Data Parameters
NAME                  LY129
EXPNO                     2
PROCNO                    1

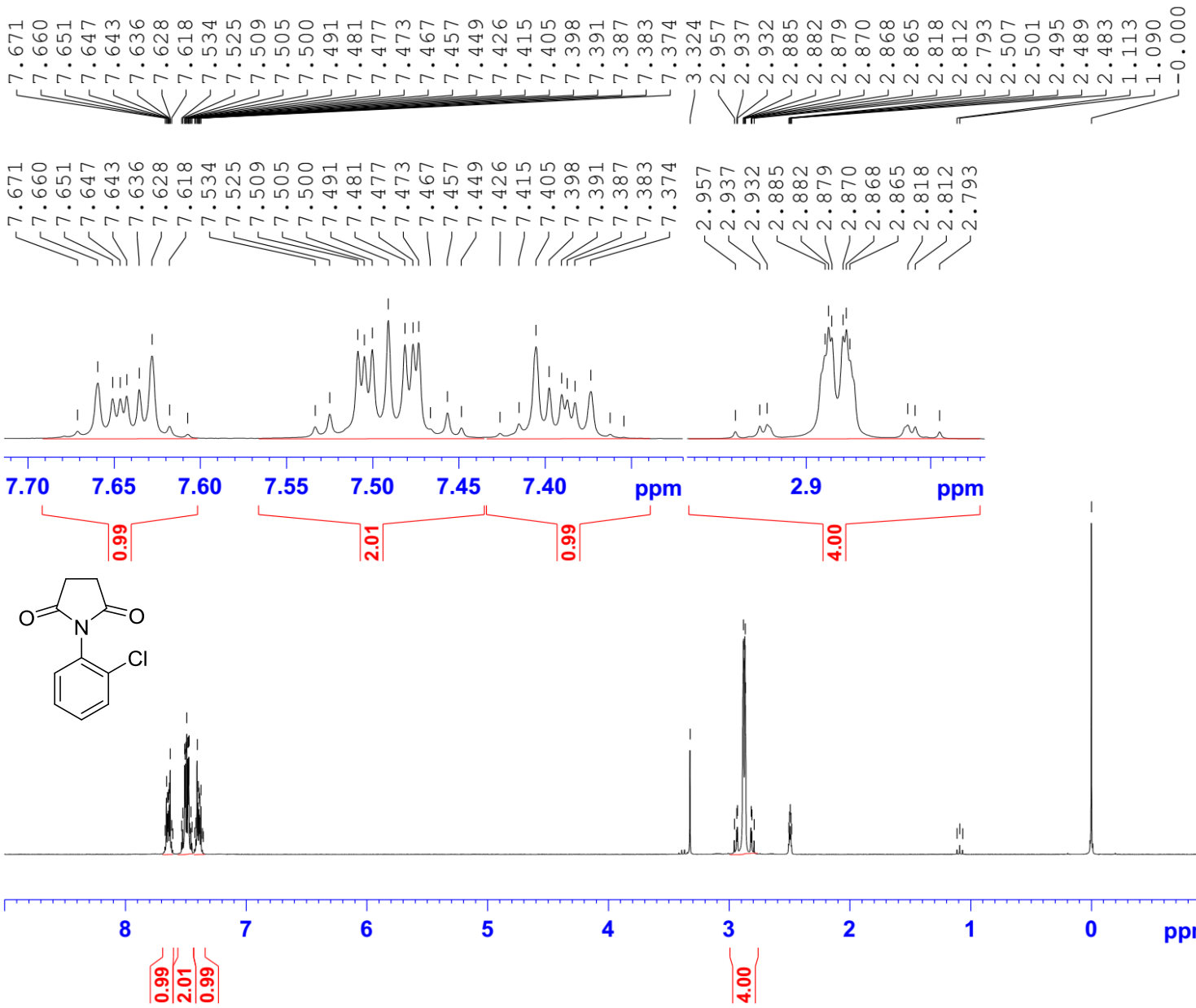
F2 - Acquisition Parameters
Date_              20171212
Time                  18.53
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                    65536
SOLVENT                DMSO
NS                     3072
DS                        4
SWH               24414.063 Hz
FIDRES             0.372529 Hz
AQ                 1.3421773 sec
RG                   501.187
DW                    20.480 usec
DE                     6.50 usec
TE                    300.2 K
D1                 2.00000000 sec
D11                0.03000000 sec
D31                0.00001500 sec
D40                0.00439029 sec
L4                        37
L5                        53
P32                   98.00 usec
TD0                       3

======== CHANNEL f1 ========
SFO1              75.4828392 MHz
NUC1                      13C
P1                    15.00 usec
PLW1             22.00000000 W

======== CHANNEL f2 ========
SFO2             300.1612006 MHz
NUC2                      1H
CPDPRG[2              waltz16
PCPD2                 98.00 usec
PLW2              9.30000019 W
PLW12             0.29359001 W
PLW13             0.20359001 W

F2 - Processing parameters
SI                        32768
SF                75.4753332 MHz
WDW                       EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

N-(2-chlorophenyl)succinimide (4c)



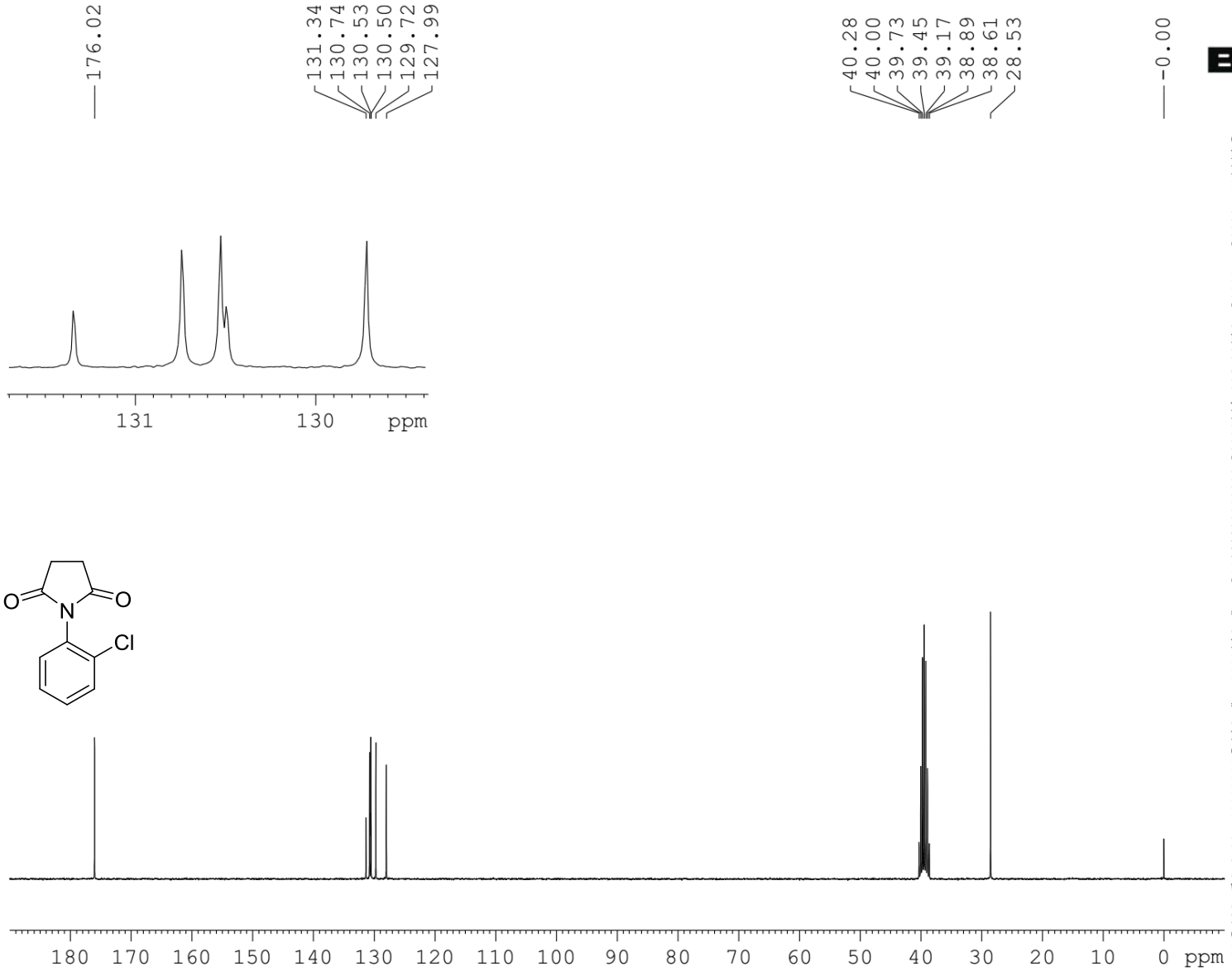

```
Current Data Parameters
NAME                  LY142
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20171225
Time                  17.13
INSTRUM         FOURIER300
PROBHD     5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       16
DS                        2
SWH                6103.516 Hz
FIDRES            0.093132 Hz
AQ                5.3687091 sec
RG                   31.623
DW                   81.920 usec
DE                    6.50 usec
TE                   300.1 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1          300.1618536 MHz
NUC1                     1H
P1                    13.50 usec
PLW1           9.30000019 W

F2 - Processing parameters
SI                    65536
SF            300.1600023 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

N-(2-chlorophenyl)succinimide (4c)



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```
Current Data Parameters
NAME                  LY142
EXPNO                     2
PROCNO                    1

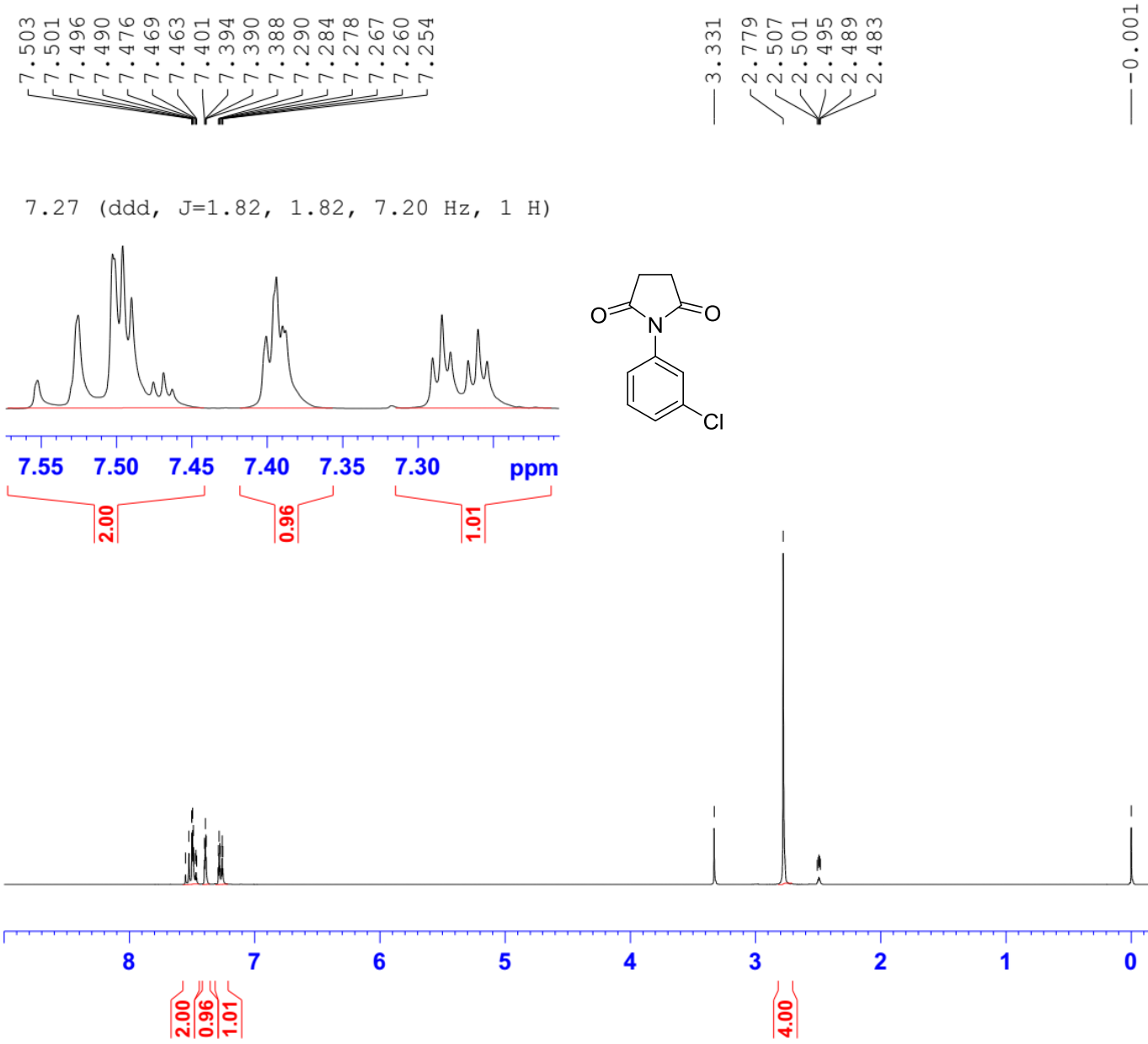
F2 - Acquisition Parameters
Date_              20171225
Time                  19.17
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT               DMSO
NS                    2048
DS                       4
SWH              24414.063 Hz
FIDRES            0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                 20.480 usec
DE                  6.50 usec
TE                  300.2 K
D1              2.00000000 sec
D11             0.03000000 sec
D31             0.00001500 sec
D40             0.00439029 sec
L4                       37
L5                       53
P32                98.00 usec
TD0                      2

======== CHANNEL f1 ========
SFO1            75.4828392 MHz
NUC1                   13C
P1                  15.00 usec
PLW1           22.00000000 W

======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                   1H
CPDPRG[2            waltz16
PCPD2               98.00 usec
PLW2            9.30000019 W
PLW12           0.29359001 W
PLW13           0.20359001 W

F2 - Processing parameters
SI                    32768
SF              75.4753349 MHz
WDW                      EM
SSB         0
LB                   1.00 Hz
GB          0
PC                   1.40
```

N-(3-chlorophenyl)succinimide (4d)



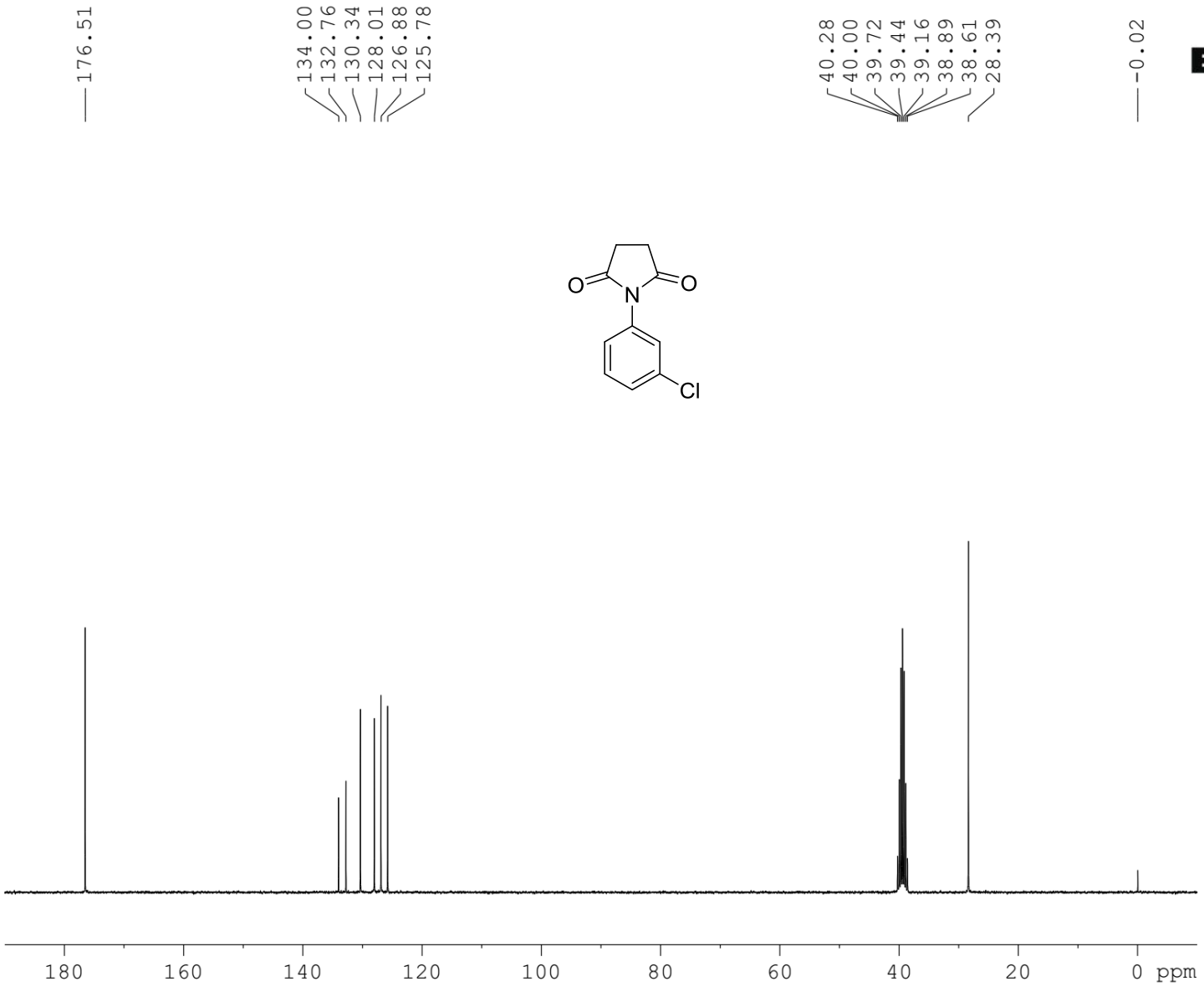

```
Current Data Parameters
NAME                  LY133
EXPNO                     3
PROCNO                    1

F2 - Acquisition Parameters
Date_              20171216
Time                  17.18
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       16
DS                        2
SWH                6103.516 Hz
FIDRES            0.093132 Hz
AQ                5.3687091 sec
RG                   31.623
DW                   81.920 usec
DE                    6.50 usec
TE                   299.9 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1             300.1618536 MHz
NUC1                       1H
P1                    13.50 usec
PLW1              9.30000019 W

F2 - Processing parameters
SI                        65536
SF               300.1600026 MHz
WDW                        EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

N-(3-chlorophenyl)succinimide (4d)



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```
Current Data Parameters
NAME                  LY133
EXPNO                     2
PROCNO                    1

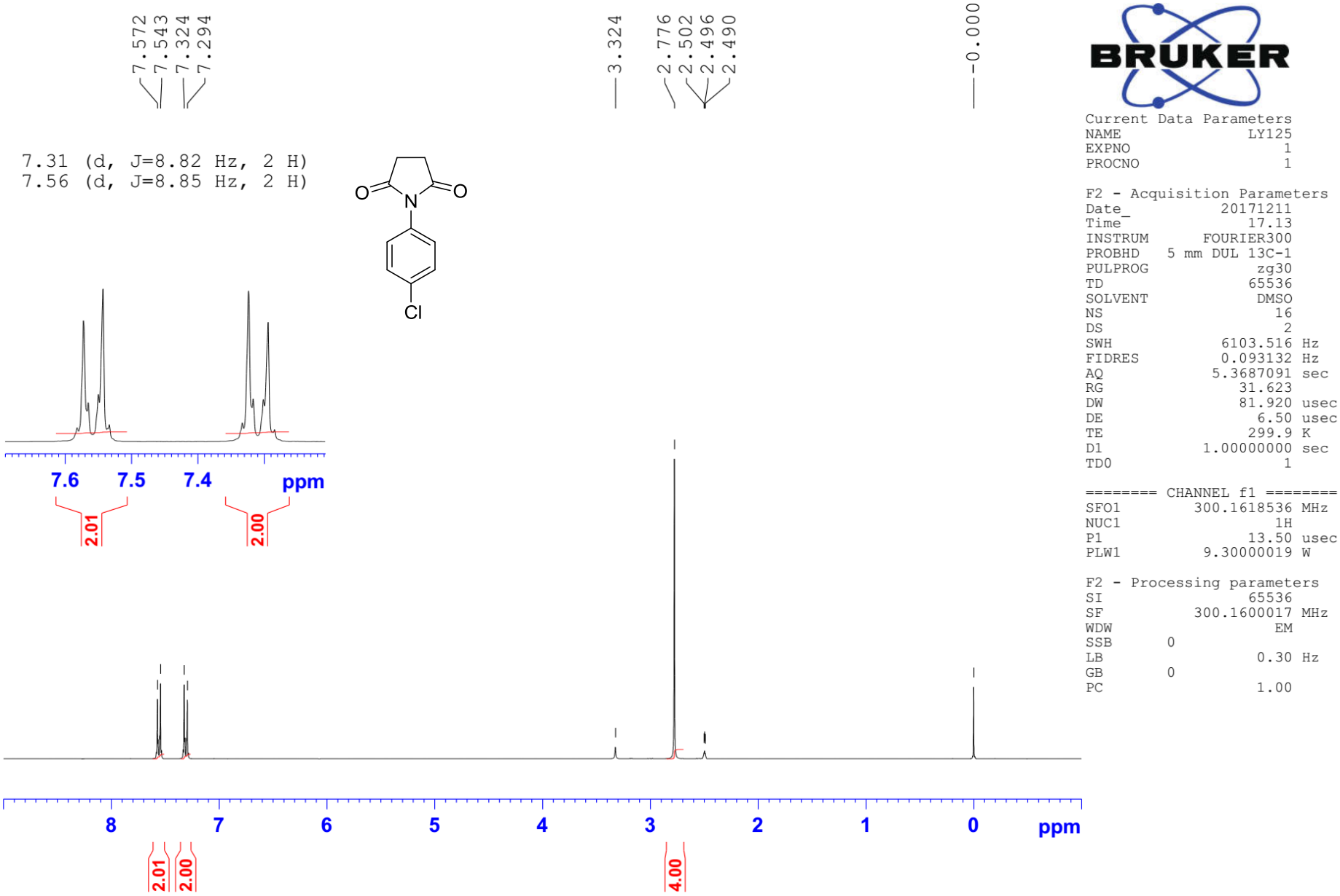
F2 - Acquisition Parameters
Date_              20171215
Time                   7.39
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                     1024
DS                        4
SWH              24414.063 Hz
FIDRES            0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                   20.480 usec
DE                    6.50 usec
TE                   300.1 K
D1             2.00000000 sec
D11            0.03000000 sec
D31            0.00001500 sec
D40            0.00439029 sec
L4                       37
L5                       53
P32                   98.00 usec
TD0                       1

======== CHANNEL f1 ========
SFO1           75.4828392 MHz
NUC1                   13C
P1                    15.00 usec
PLW1          22.00000000 W

======== CHANNEL f2 ========
SFO2          300.1612006 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2                 98.00 usec
PLW2           9.30000019 W
PLW12          0.29359001 W
PLW13          0.20359001 W

F2 - Processing parameters
SI                    32768
SF             75.4753350 MHz
WDW                      EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```

N-(4-chlorophenyl)succinimide (4e)



BRUKER

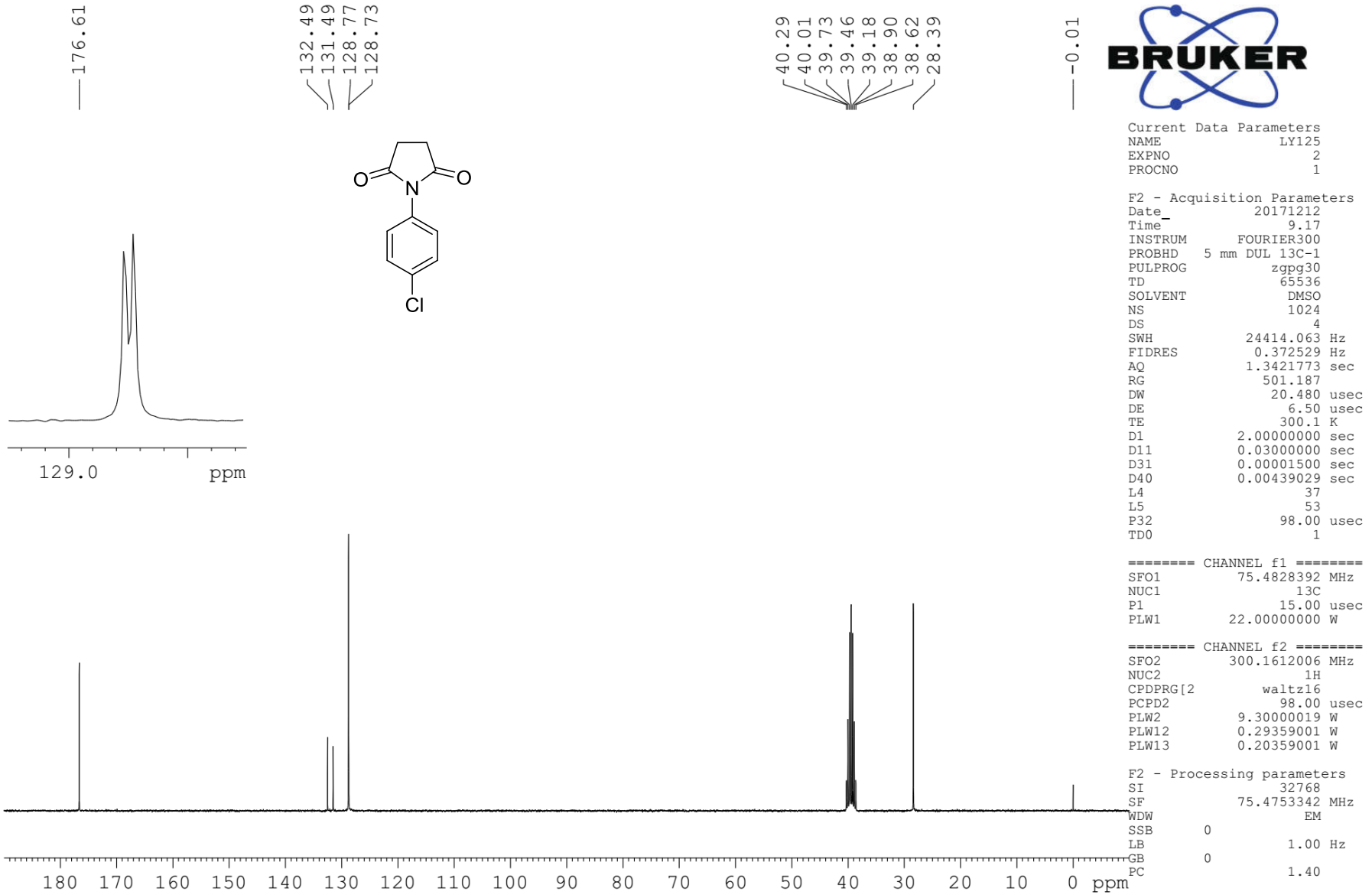
```
Current Data Parameters
NAME                  LY125
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20171211
Time                  17.13
INSTRUM          FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       16
DS                        2
SWH                6103.516 Hz
FIDRES             0.093132 Hz
AQ                 5.3687091 sec
RG                    31.623
DW                    81.920 usec
DE                     6.50 usec
TE                    299.9 K
D1                 1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1            300.1618536 MHz
NUC1                      1H
P1                    13.50 usec
PLW1            9.30000019 W

F2 - Processing parameters
SI                    65536
SF              300.1600017 MHz
WDW                      EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

N-(4-chlorophenyl)succinimide (4e)




```
Current Data Parameters
NAME                  LY125
EXPNO                     2
PROCNO                    1

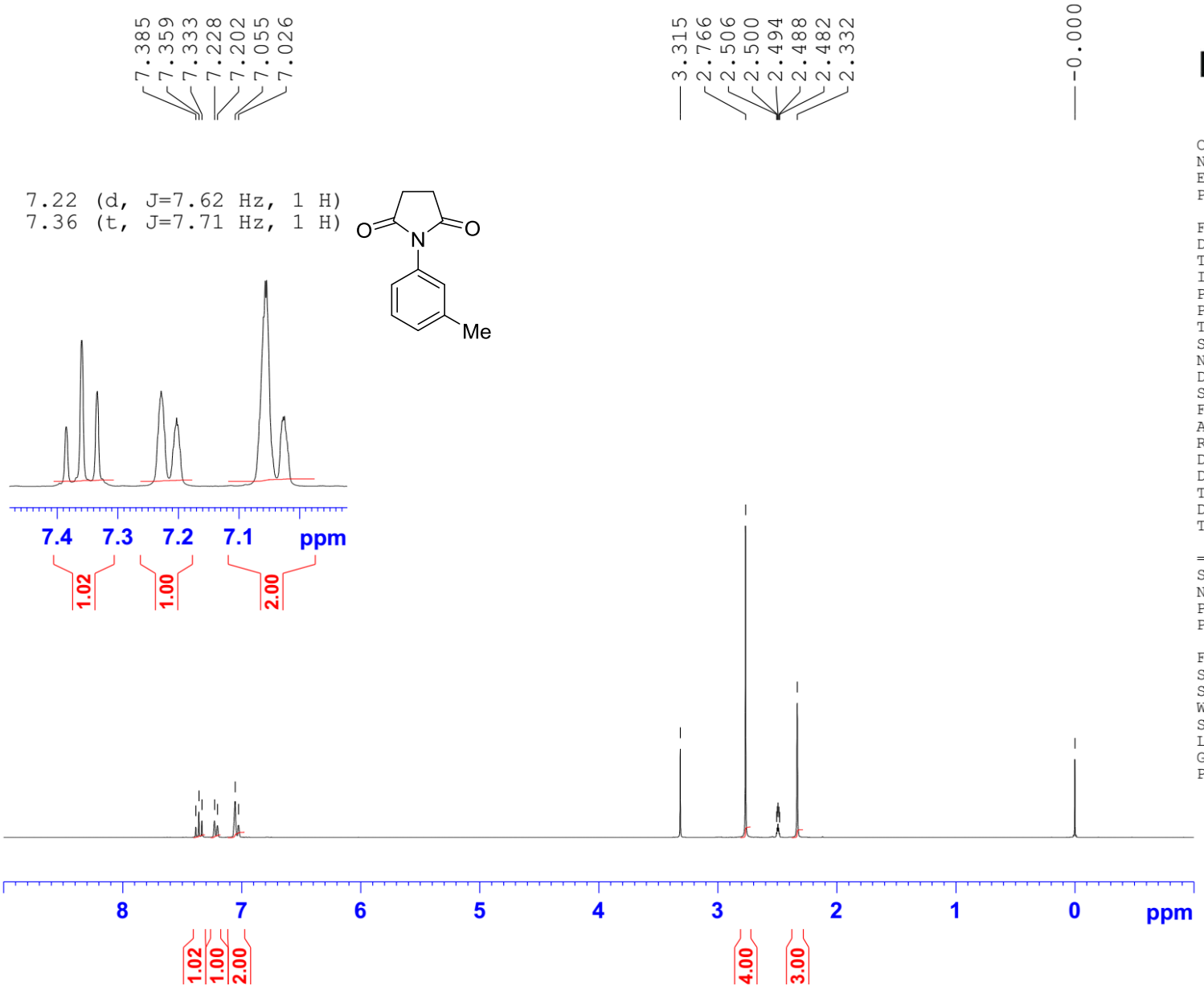
F2 - Acquisition Parameters
Date_              20171212
Time                   9.17
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                     1024
DS                        4
SWH              24414.063 Hz
FIDRES               0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                   20.480 usec
DE                    6.50 usec
TE                   300.1 K
D1               2.00000000 sec
D11              0.03000000 sec
D31              0.00001500 sec
D40              0.00439029 sec
L4                       37
L5                       53
P32                   98.00 usec
TD0                       1

======== CHANNEL f1 ========
SFO1            75.4828392 MHz
NUC1                    13C
P1                    15.00 usec
PLW1           22.00000000 W

======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2                 98.00 usec
PLW2            9.30000019 W
PLW12           0.29359001 W
PLW13           0.20359001 W

F2 - Processing parameters
SI                      32768
SF               75.4753342 MHz
WDW                        EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

N-(3-methylphenyl)succinimide (4f)



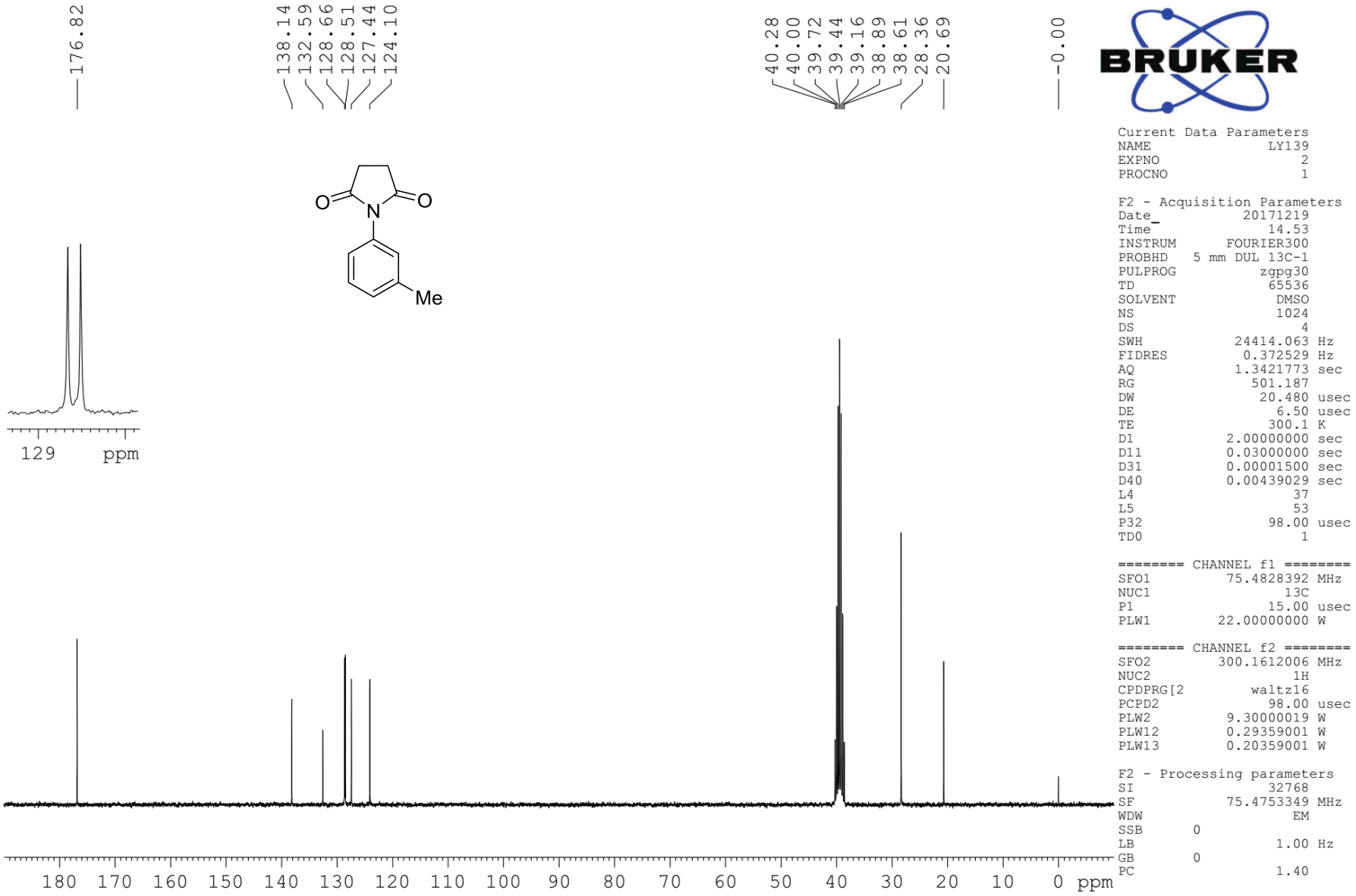

```
Current Data Parameters
NAME                 LY139
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20171219
Time                 13.20
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                      16
DS                       2
SWH              6103.516 Hz
FIDRES           0.093132 Hz
AQ               5.3687091 sec
RG                  31.623
DW                  81.920 usec
DE                   6.50 usec
TE                  300.0 K
D1               1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          300.1618536 MHz
NUC1                    1H
P1                   13.50 usec
PLW1           9.30000019 W

F2 - Processing parameters
SI                   65536
SF            300.1600026 MHz
WDW                     EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```

N-(3-methylphenyl)succinimide (4f)



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```
Current Data Parameters
NAME                  LY139
EXPNO                     2
PROCNO                    1

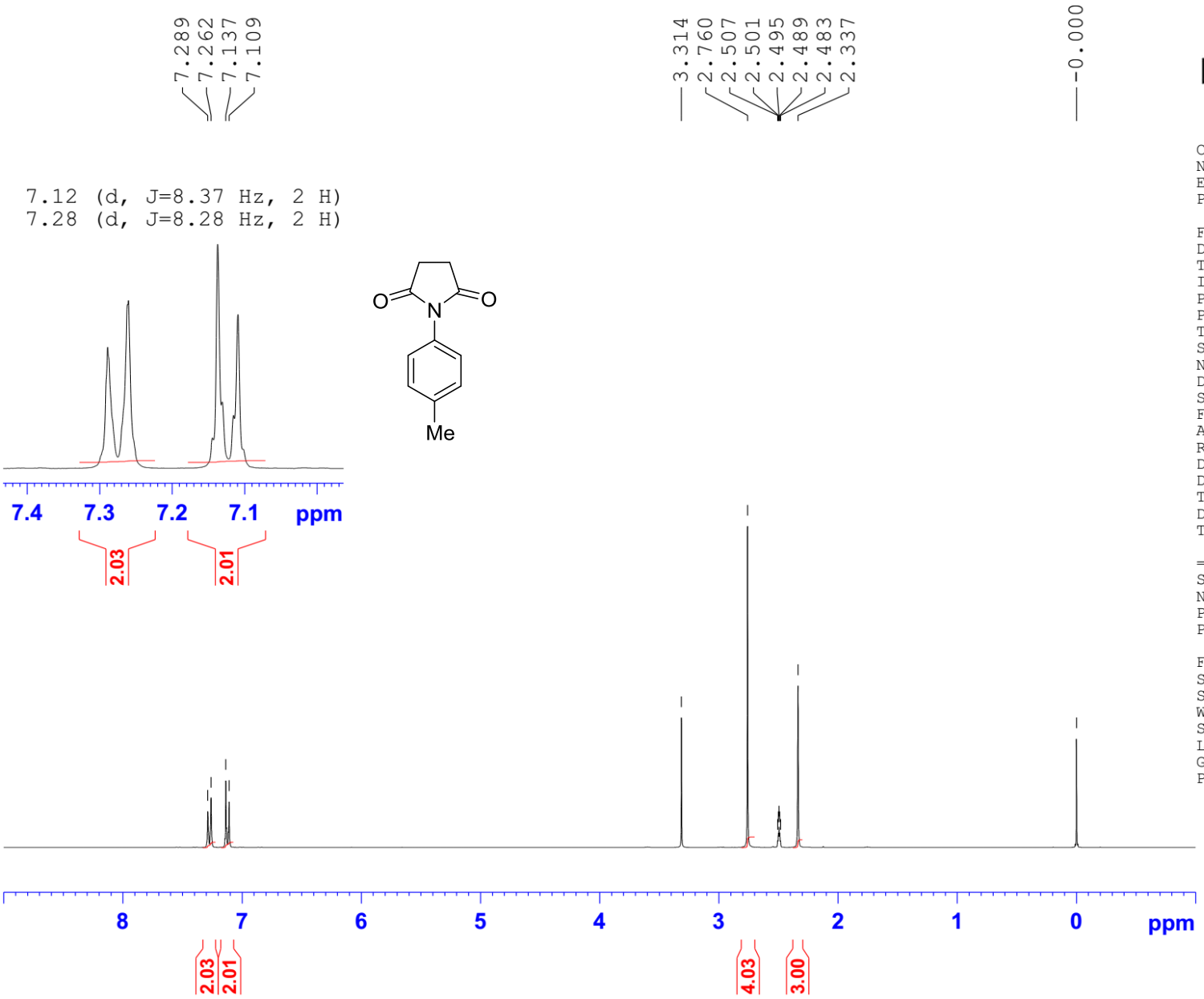
F2 - Acquisition Parameters
Date_              20171219
Time                  14.53
INSTRUM       FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                    65536
SOLVENT                DMSO
NS                     1024
DS                        4
SWH              24414.063 Hz
FIDRES            0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                   20.480 usec
DE                    6.50 usec
TE                   300.1 K
D1               2.00000000 sec
D11              0.03000000 sec
D31              0.00001500 sec
D40              0.00439029 sec
L4                       37
L5                       53
P32                   98.00 usec
TD0                       1

======== CHANNEL f1 ========
SFO1            75.4828392 MHz
NUC1                    13C
P1                    15.00 usec
PLW1           22.00000000 W

======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2                 98.00 usec
PLW2            9.30000019 W
PLW12           0.29359001 W
PLW13           0.20359001 W

F2 - Processing parameters
SI                    32768
SF              75.4753349 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

N-(4-methylphenyl)succinimide (4g)



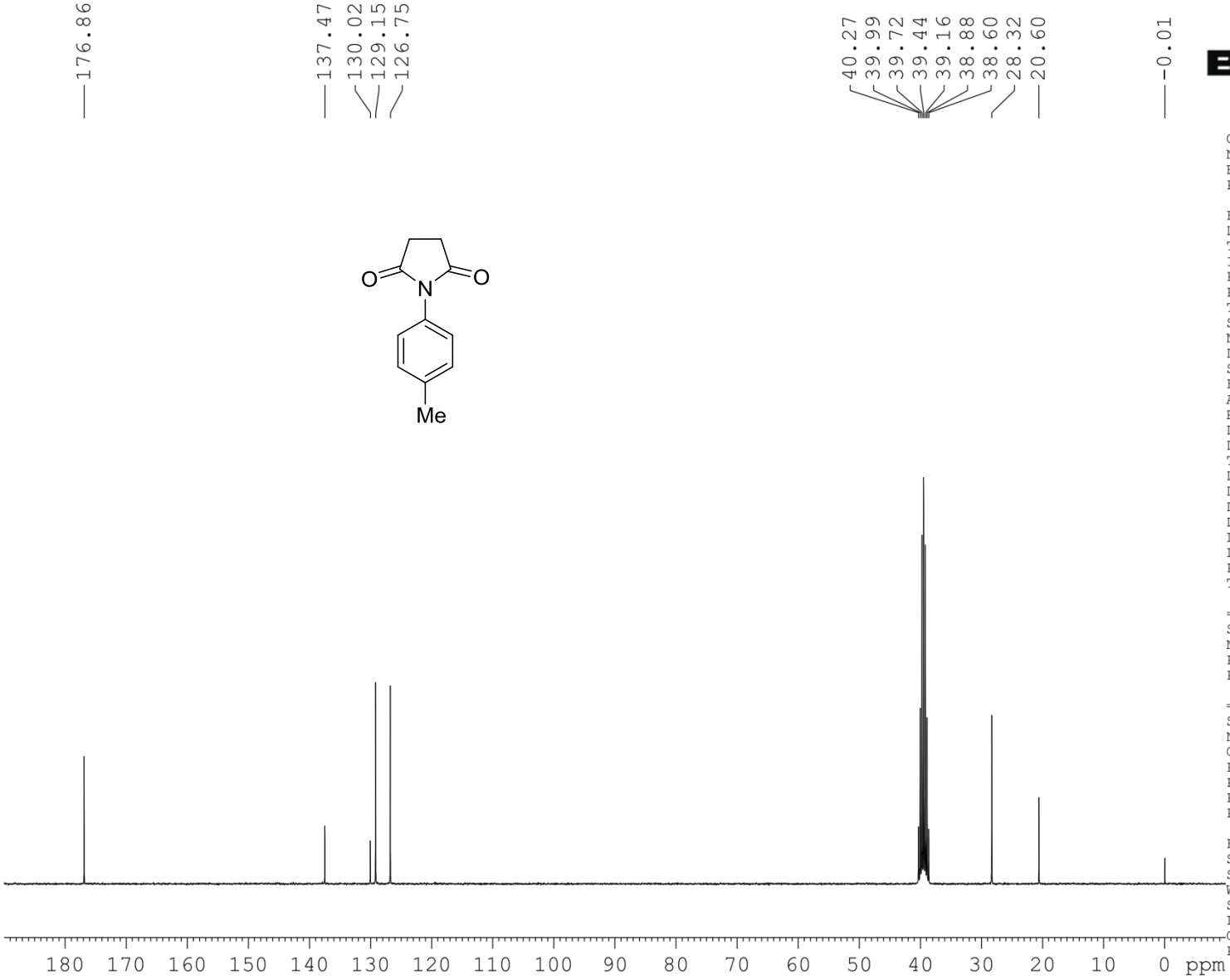

```
Current Data Parameters
NAME                  LY124
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20171216
Time                  17.36
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       16
DS                        2
SWH                6103.516 Hz
FIDRES            0.093132 Hz
AQ                5.3687091 sec
RG                   53.7088
DW                  81.920 usec
DE                   6.50 usec
TE                  300.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1          300.1618536 MHz
NUC1                     1H
P1                    13.50 usec
PLW1           9.30000019 W

F2 - Processing parameters
SI                    65536
SF            300.1600023 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

N-(4-methylphenyl)succinimide (4g)



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```
Current Data Parameters
NAME                  LY124
EXPNO                     2
PROCNO                    1

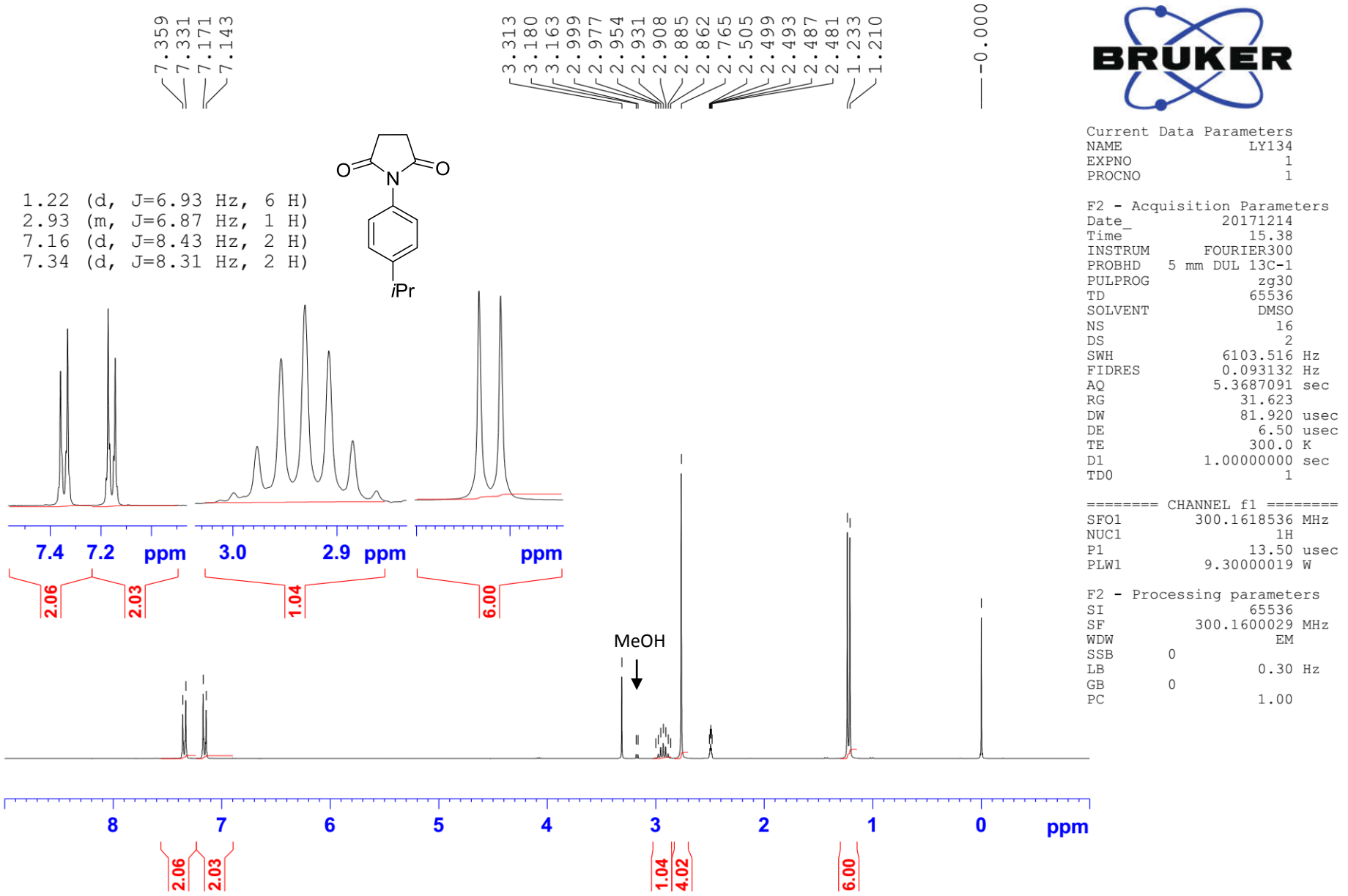
F2 - Acquisition Parameters
Date_              20171216
Time                  18.14
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT               DMSO
NS                    4096
DS                       4
SWH              24414.063 Hz
FIDRES            0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                   20.480 usec
DE                    6.50 usec
TE                   300.1 K
D1                2.00000000 sec
D11               0.03000000 sec
D31               0.00001500 sec
D40               0.00439029 sec
L4                       37
L5                       53
P32                  98.00 usec
TD0                      4

======== CHANNEL f1 ========
SFO1             75.4828392 MHz
NUC1                    13C
P1                   15.00 usec
PLW1            22.00000000 W

======== CHANNEL f2 ========
SFO2            300.1612006 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                98.00 usec
PLW2             9.30000019 W
PLW12            0.29359001 W
PLW13            0.20359001 W

F2 - Processing parameters
SI                      32768
SF               75.4753352 MHz
WDW                        EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

N-(4-isopropylphenyl)succinimide (4h)



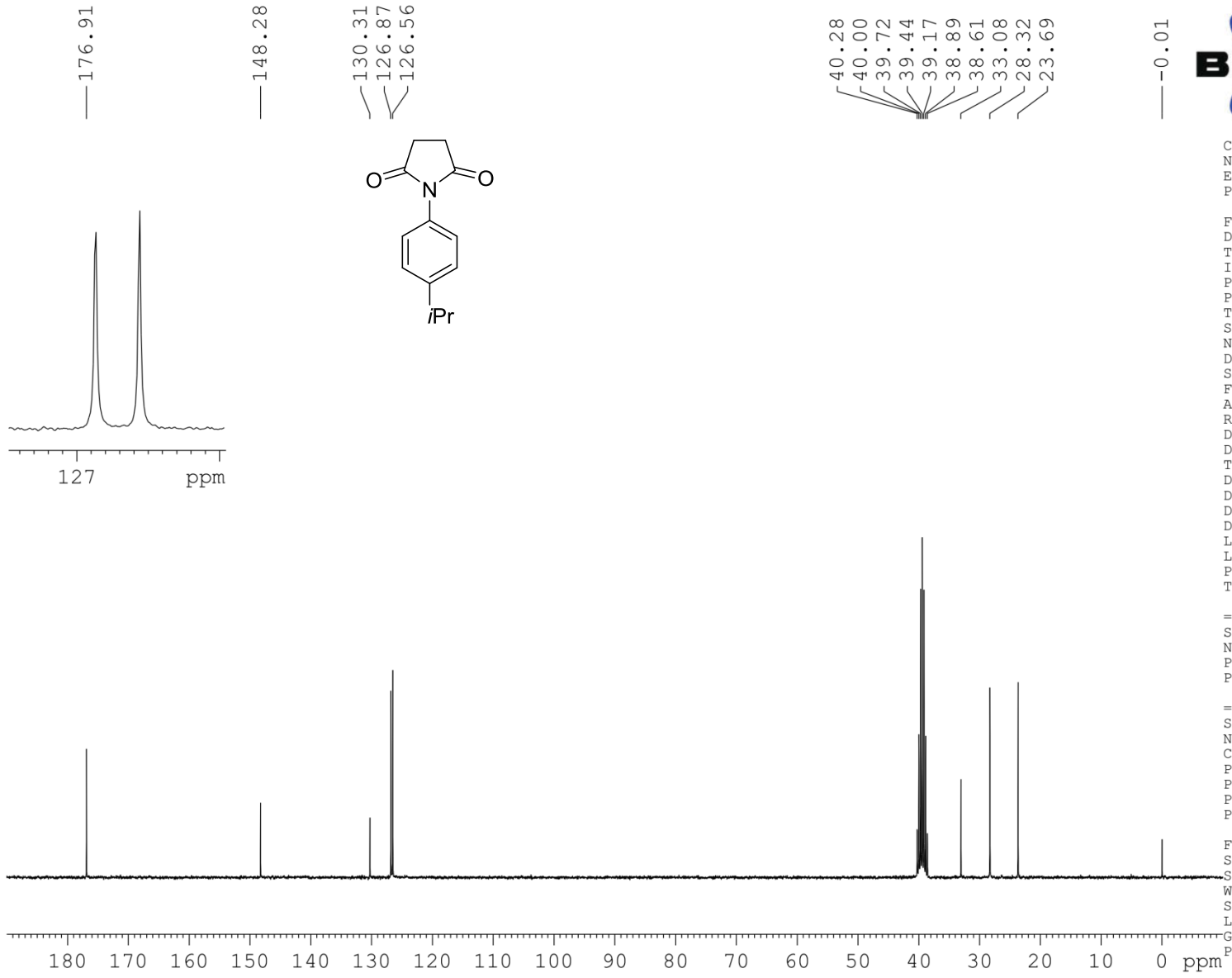

```
Current Data Parameters
NAME                  LY134
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20171214
Time                  15.38
INSTRUM          FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT               DMSO
NS                       16
DS                        2
SWH                6103.516 Hz
FIDRES            0.093132 Hz
AQ                5.3687091 sec
RG                   31.623
DW                   81.920 usec
DE                    6.50 usec
TE                   300.0 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           300.1618536 MHz
NUC1                     1H
P1                    13.50 usec
PLW1            9.30000019 W

F2 - Processing parameters
SI                   65536
SF             300.1600029 MHz
WDW                     EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```

N-(4-isopropylphenyl)succinimide (4h)



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```
Current Data Parameters
NAME                  LY134
EXPNO                     2
PROCNO                    1

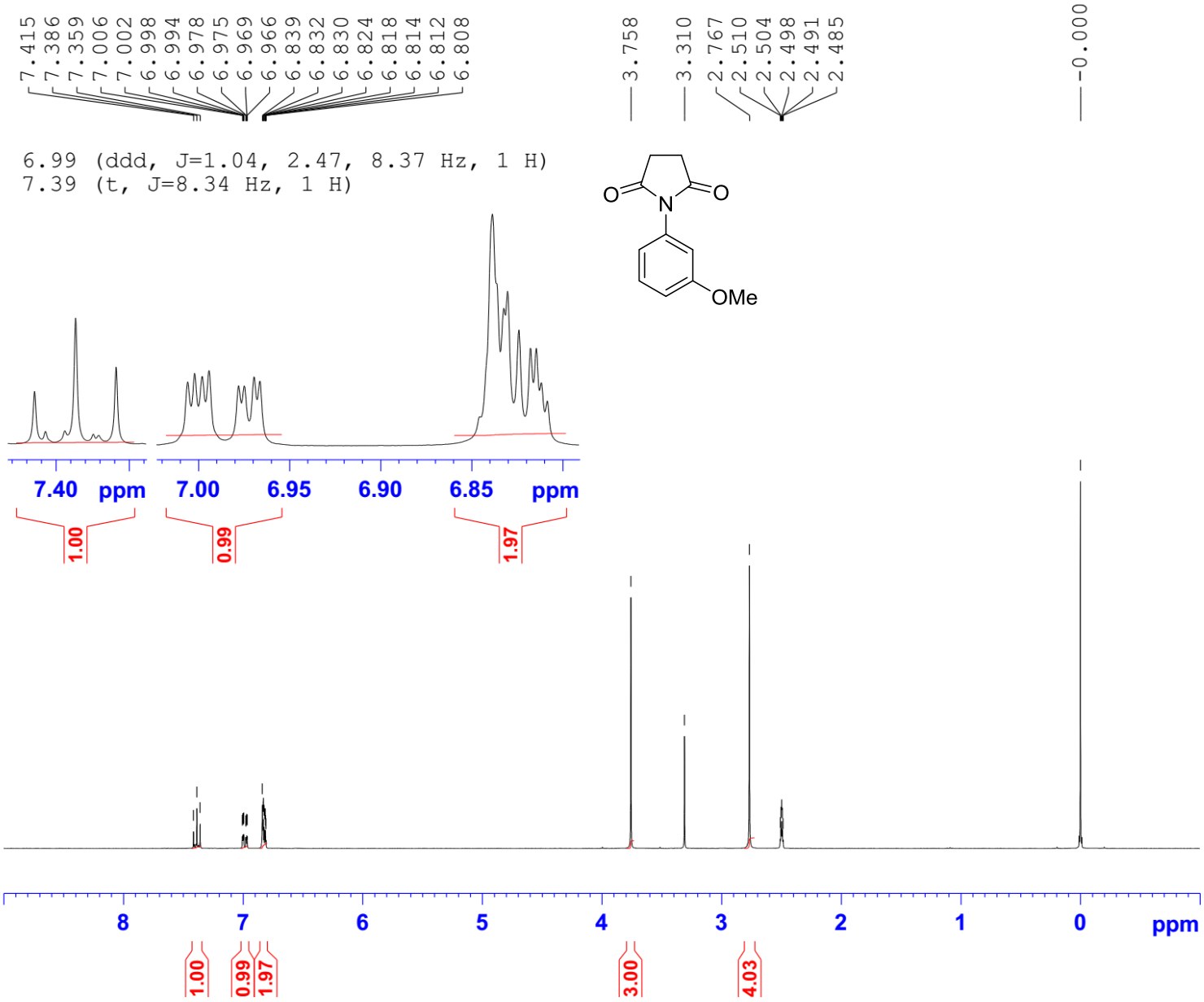
F2 - Acquisition Parameters
Date_              20171214
Time                  16.08
INSTRUM          FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                    65536
SOLVENT                DMSO
NS                     1024
DS                        4
SWH              24414.063 Hz
FIDRES            0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                   20.480 usec
DE                    6.50 usec
TE                   300.1 K
D1             2.00000000 sec
D11            0.03000000 sec
D31            0.00001500 sec
D40            0.00439029 sec
L4                       37
L5                       53
P32                  98.00 usec
TD0                       1

======== CHANNEL f1 ========
SFO1            75.4828392 MHz
NUC1                   13C
P1                   15.00 usec
PLW1           22.00000000 W

======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                   1H
CPDPRG[2            waltz16
PCPD2                98.00 usec
PLW2            9.30000019 W
PLW12           0.29359001 W
PLW13           0.20359001 W

F2 - Processing parameters
SI                    32768
SF              75.4753350 MHz
WDW                      EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

N-(3-methoxyphenyl)succinimide (4i)



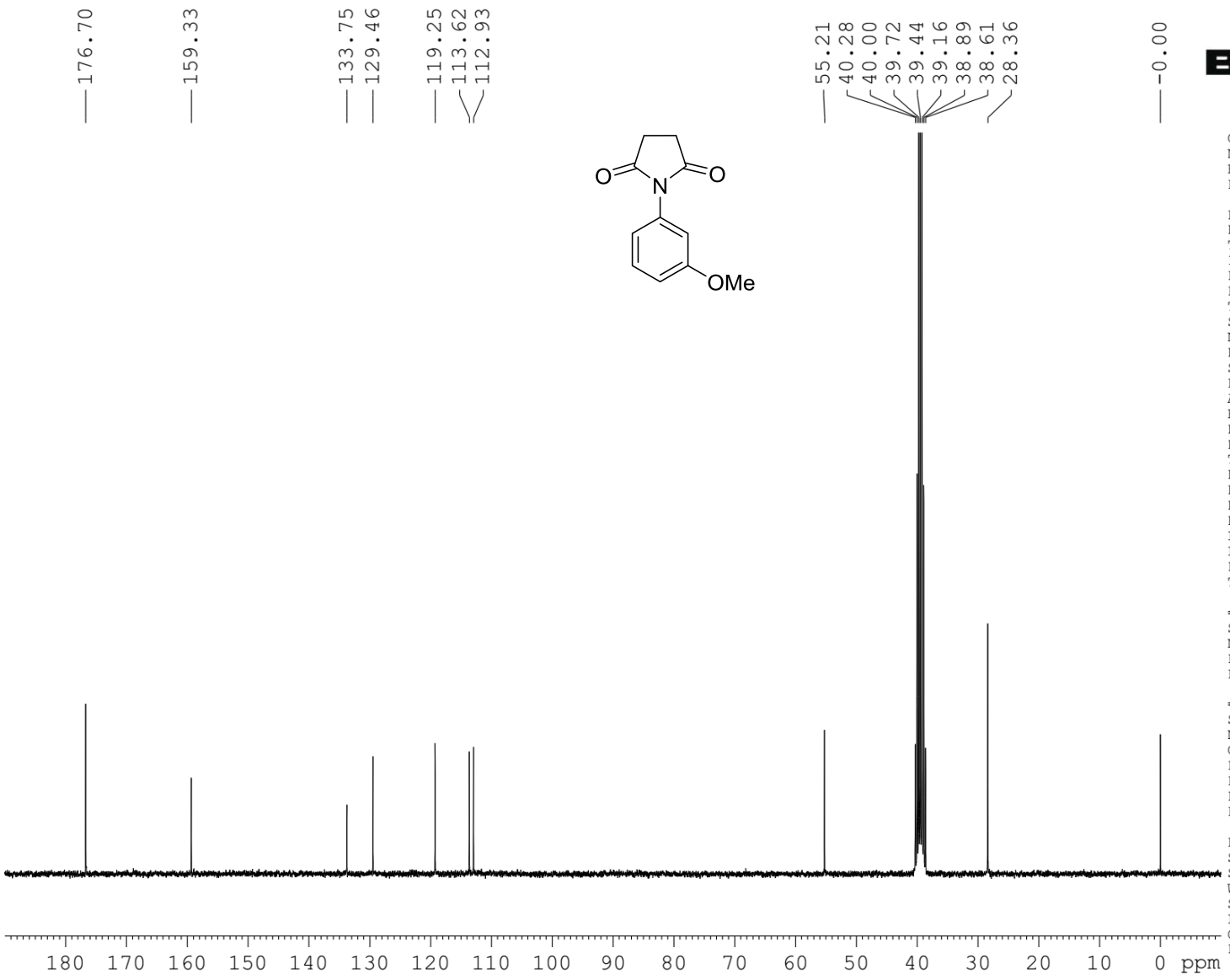

```
Current Data Parameters
NAME                  LY141
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20171225
Time                  17.08
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       16
DS                        2
SWH               6103.516 Hz
FIDRES            0.093132 Hz
AQ                5.3687091 sec
RG                   79.5788
DW                   81.920 usec
DE                    6.50 usec
TE                   300.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           300.1618536 MHz
NUC1                      1H
P1                    13.50 usec
PLW1           9.30000019 W

F2 - Processing parameters
SI                    65536
SF             300.1600014 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

N-(3-methoxyphenyl)succinimide (4i)



BRUKER

```
Current Data Parameters
NAME                 LY141
EXPNO                    2
PROCNO                   1

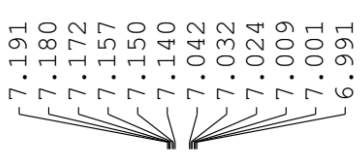
F2 - Acquisition Parameters
Date_             20171225
Time                 17.18
INSTRUM       FOURIER300
PROBHD   5 mm DUL 13C-1
PULPROG            zgpg30
TD                   65536
SOLVENT                DMSO
NS                     2048
DS                        4
SWH              24414.063 Hz
FIDRES               0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                   20.480 usec
DE                    6.50 usec
TE                   300.1 K
D1              2.00000000 sec
D11             0.03000000 sec
D31             0.00001500 sec
D40             0.00439029 sec
L4                       37
L5                       53
P32                   98.00 usec
TD0                      2

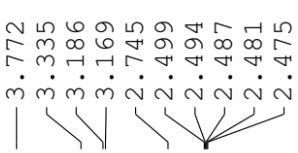
======== CHANNEL f1 ========
SFO1            75.4828392 MHz
NUC1                    13C
P1                    15.00 usec
PLW1           22.00000000 W

======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2                 98.00 usec
PLW2            9.30000019 W
PLW12           0.29359001 W
PLW13           0.20359001 W

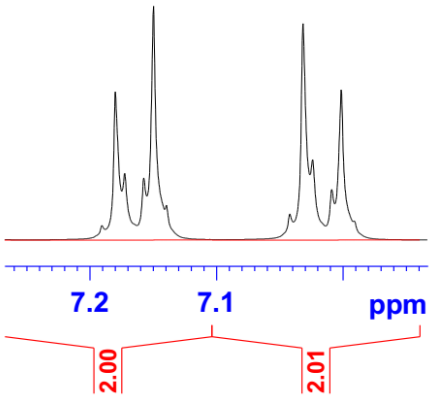
F2 - Processing parameters
SI                    32768
SF              75.4753350 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

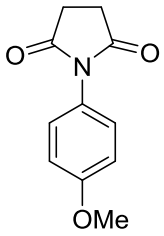
N-(4-methoxyphenyl)succinimide (4j)

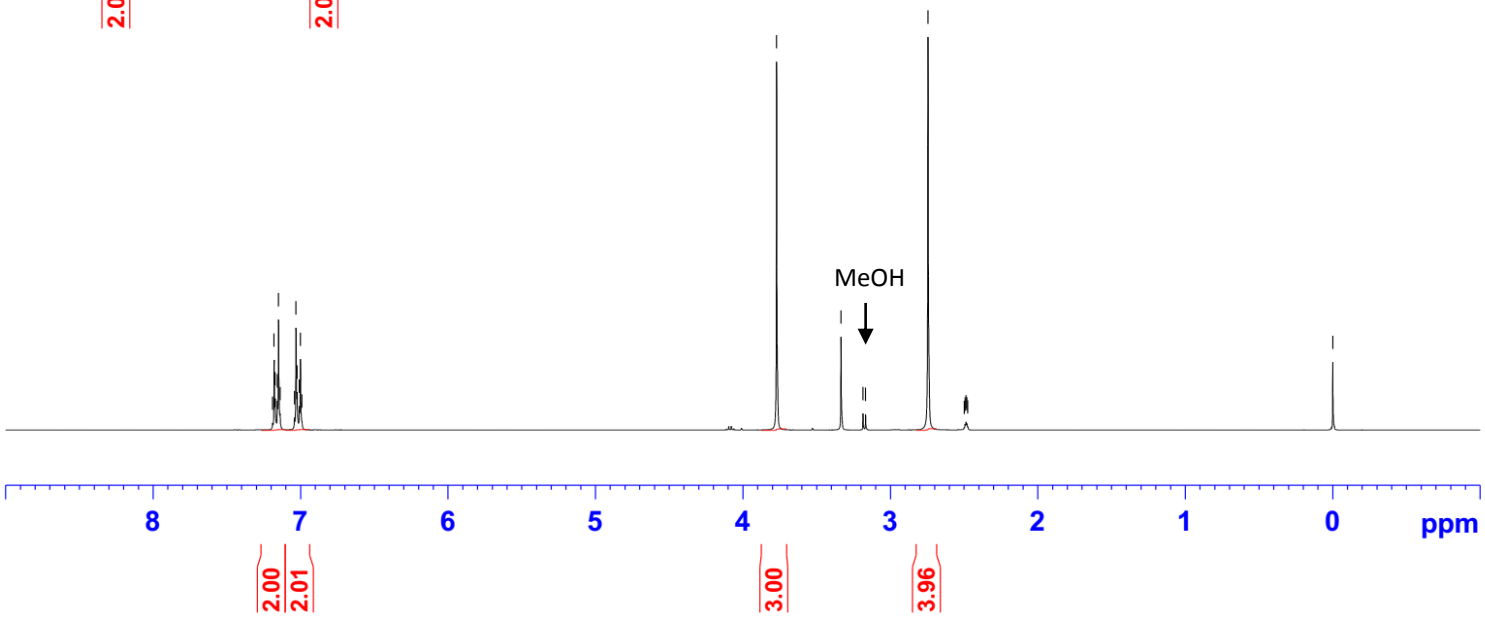




7.02 (d, J=9.06 Hz, 2 H)
7.16 (d, J=9.06 Hz, 2 H)







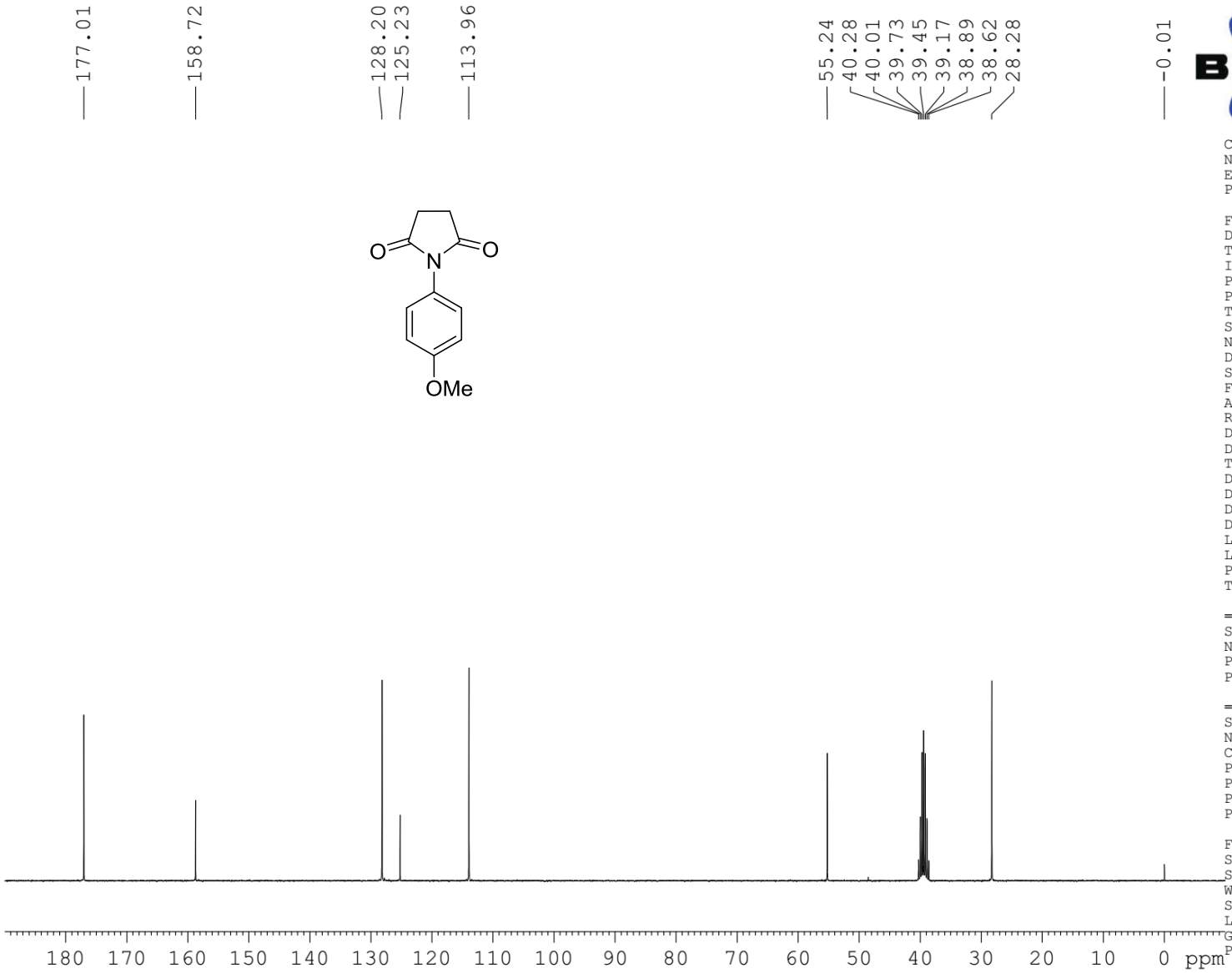

```
Current Data Parameters
NAME                  LY127
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20171216
Time                  16.51
INSTRUM          FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       16
DS                        2
SWH                6103.516 Hz
FIDRES            0.093132 Hz
AQ                5.3687091 sec
RG                  16.1049
DW                  81.920 usec
DE                   6.50 usec
TE                  300.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           300.1618536 MHz
NUC1                      1H
P1                    13.50 usec
PLW1           9.30000019 W

F2 - Processing parameters
SI                    65536
SF             300.1600047 MHz
WDW                      EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```

N-(4-methoxyphenyl)succinimide (4j)




```
Current Data Parameters
NAME                  LY127
EXPNO                     2
PROCNO                    1

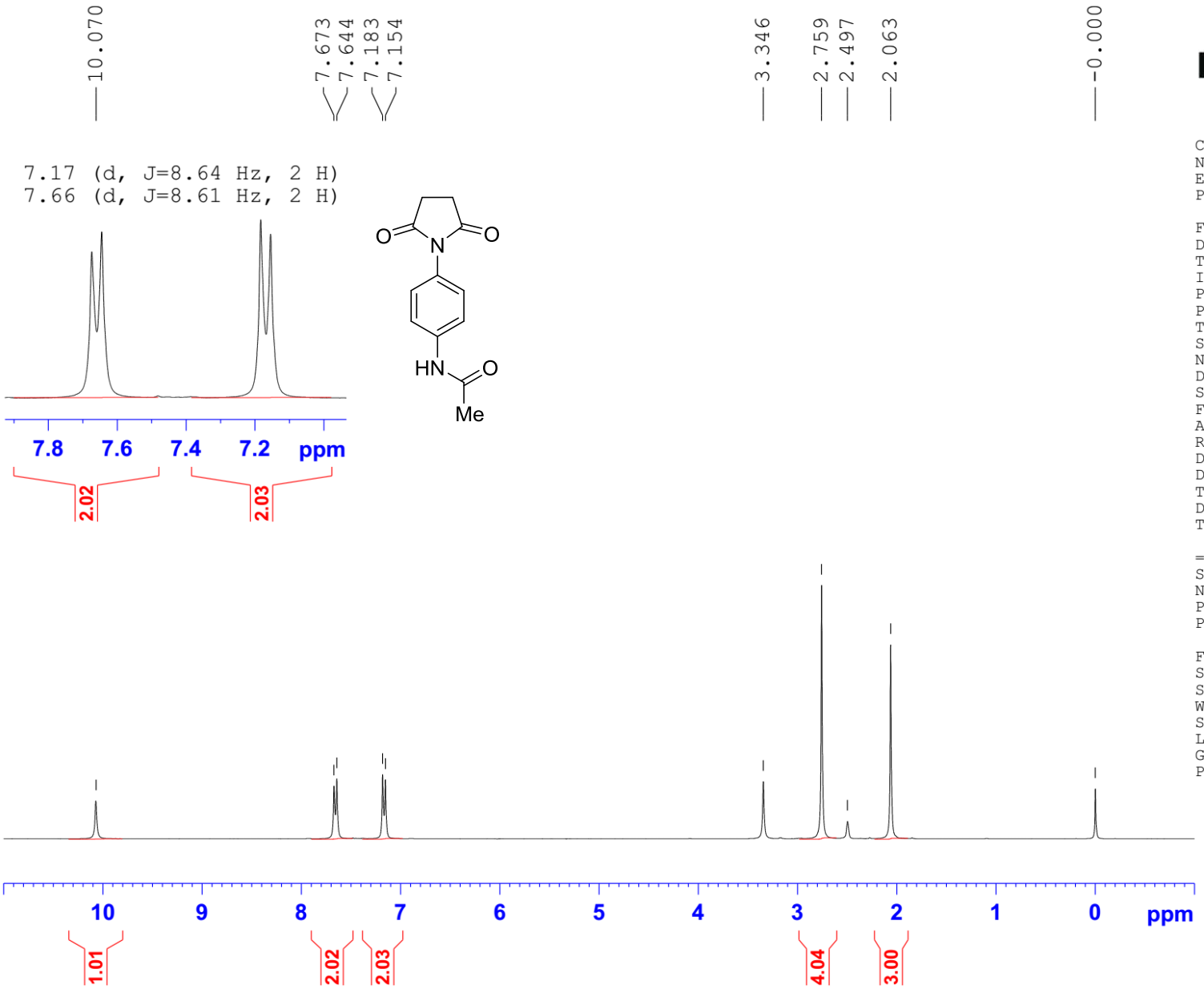
F2 - Acquisition Parameters
Date_              20171211
Time                 18.40
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG            zgpg30
TD                  65536
SOLVENT              DMSO
NS                   1024
DS                      4
SWH             24414.063 Hz
FIDRES              0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                   20.480 usec
DE                    6.50 usec
TE                   300.1 K
D1              2.00000000 sec
D11             0.03000000 sec
D31             0.00001500 sec
D40             0.00439029 sec
L4                      37
L5                      53
P32                  98.00 usec
TD0                     1

======== CHANNEL f1 ========
SFO1            75.4828392 MHz
NUC1                   13C
P1                   15.00 usec
PLW1           22.00000000 W

======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2                98.00 usec
PLW2            9.30000019 W
PLW12           0.29359001 W
PLW13           0.20359001 W

F2 - Processing parameters
SI                    32768
SF              75.4753336 MHz
WDW                      EM
SSB         0
LB                    1.00 Hz
GB          0
PC                    1.40
```

N-(4-(N-acetamide)phenyl)succinimide (4k)



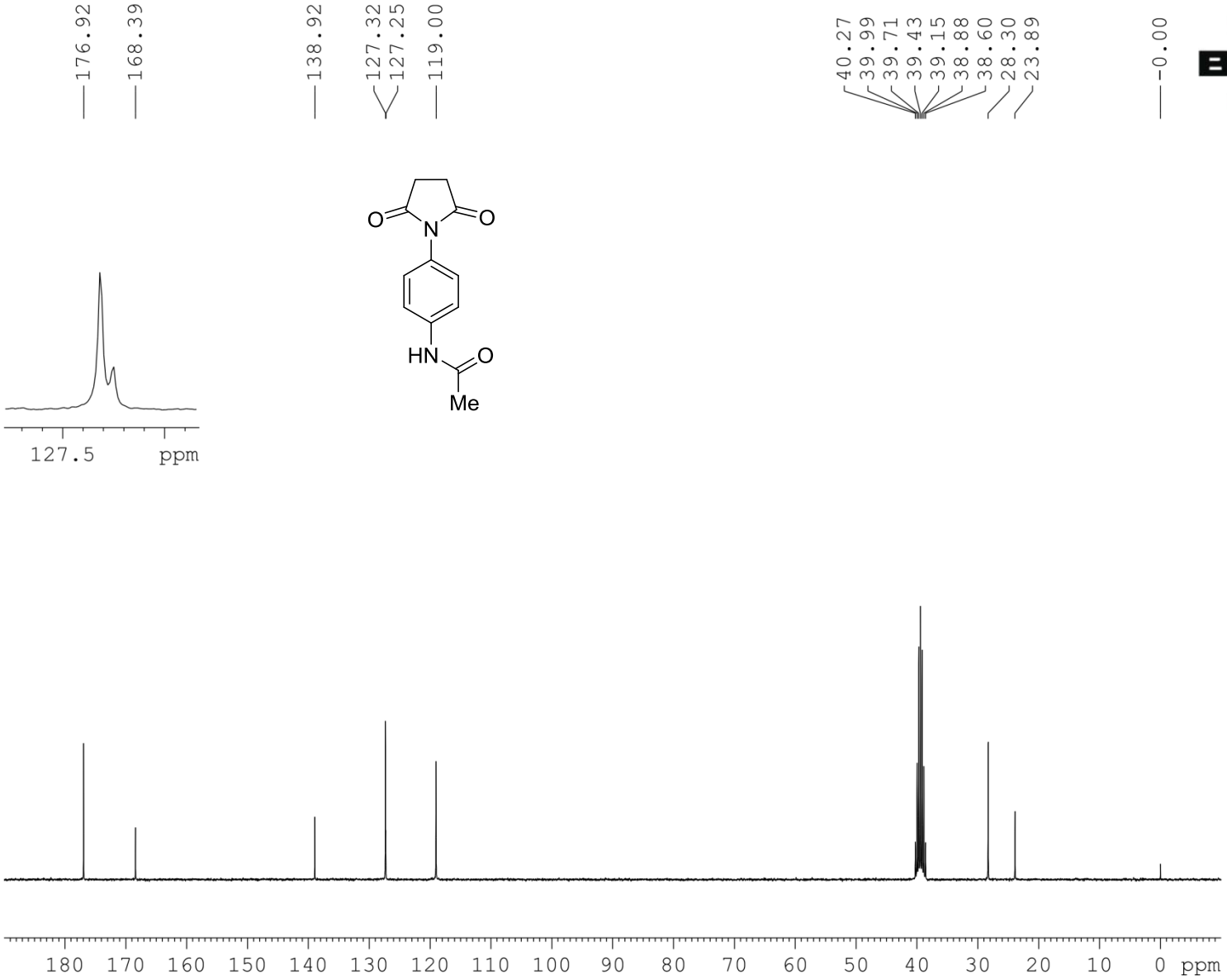

```
Current Data Parameters
NAME                  LY130
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20171213
Time                  14.44
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       16
DS                        2
SWH                6103.516 Hz
FIDRES            0.093132 Hz
AQ                5.3687091 sec
RG                   31.623
DW                   81.920 usec
DE                    6.50 usec
TE                   300.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1          300.1618536 MHz
NUC1                     1H
P1                    13.50 usec
PLW1           9.30000019 W

F2 - Processing parameters
SI                    65536
SF            300.1600017 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

N-(4-(N-acetamide)phenyl)succinimide (4k)




```
Current Data Parameters
NAME                  LY130
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20171214
Time                   9.21
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                     1024
DS                        4
SWH              24414.063 Hz
FIDRES            0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                 20.480 usec
DE                  6.50 usec
TE                  300.1 K
D1              2.00000000 sec
D11             0.03000000 sec
D31             0.00001500 sec
D40             0.00439029 sec
L4                       37
L5                       53
P32                98.00 usec
TD0                       1

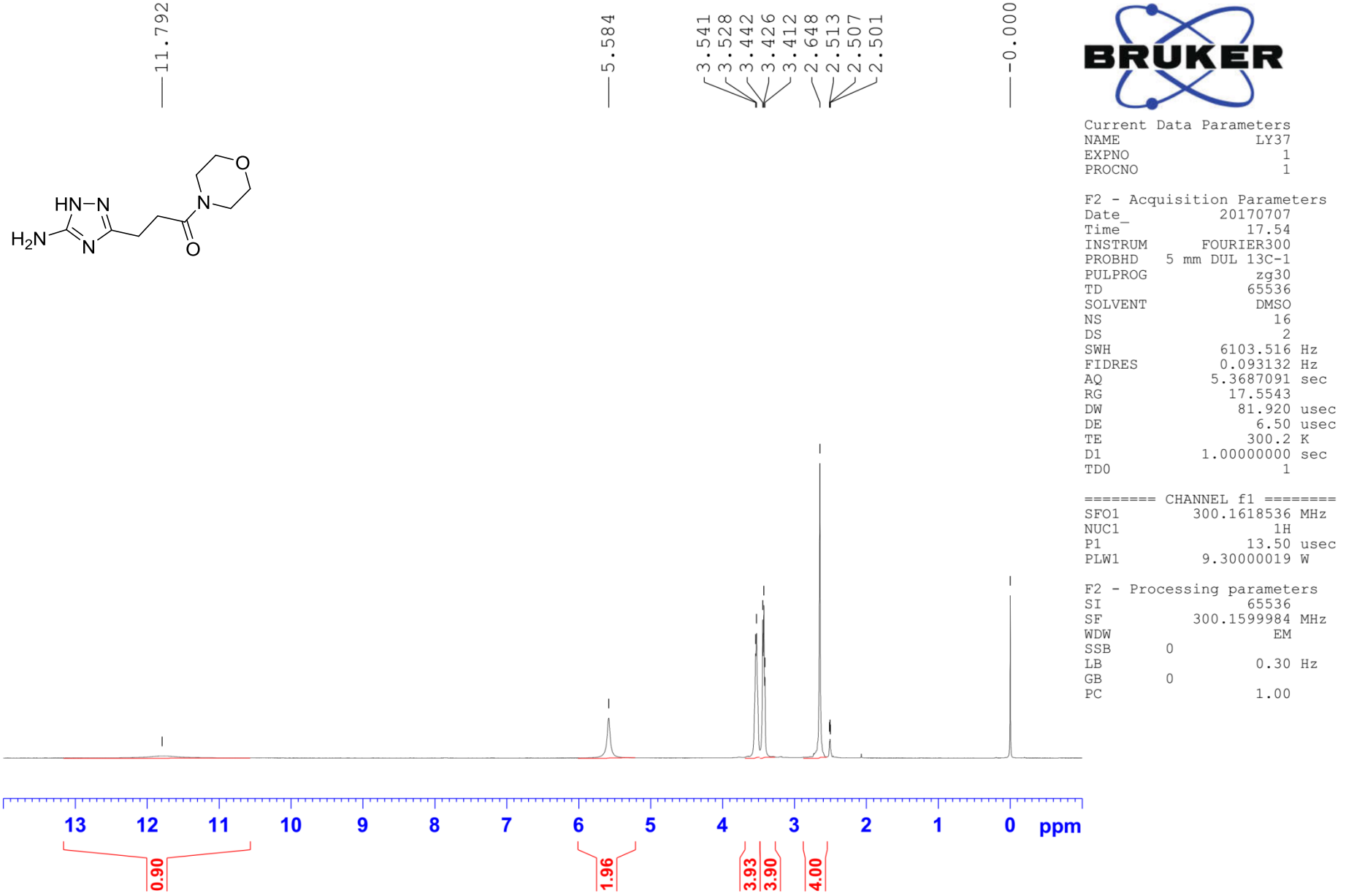
======== CHANNEL f1 ========
SFO1            75.4828392 MHz
NUC1                    13C
P1                  15.00 usec
PLW1           22.00000000 W

======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2               98.00 usec
PLW2            9.30000019 W
PLW12           0.29359001 W
PLW13           0.20359001 W

F2 - Processing parameters
SI                    32768
SF              75.4753343 MHz
WDW                      EM
SSB         0
LB                   1.00 Hz
GB          0
PC                   1.40
```

^{1}H and ^{13}C NMR spectra of 3-(5-amino-1*H*-1,2,4-triazol-3-yl)propanamides 5

3-(5-Amino-1H-1,2,4-triazol-3-yl)-1-morpholinopropan-1-one (5a)



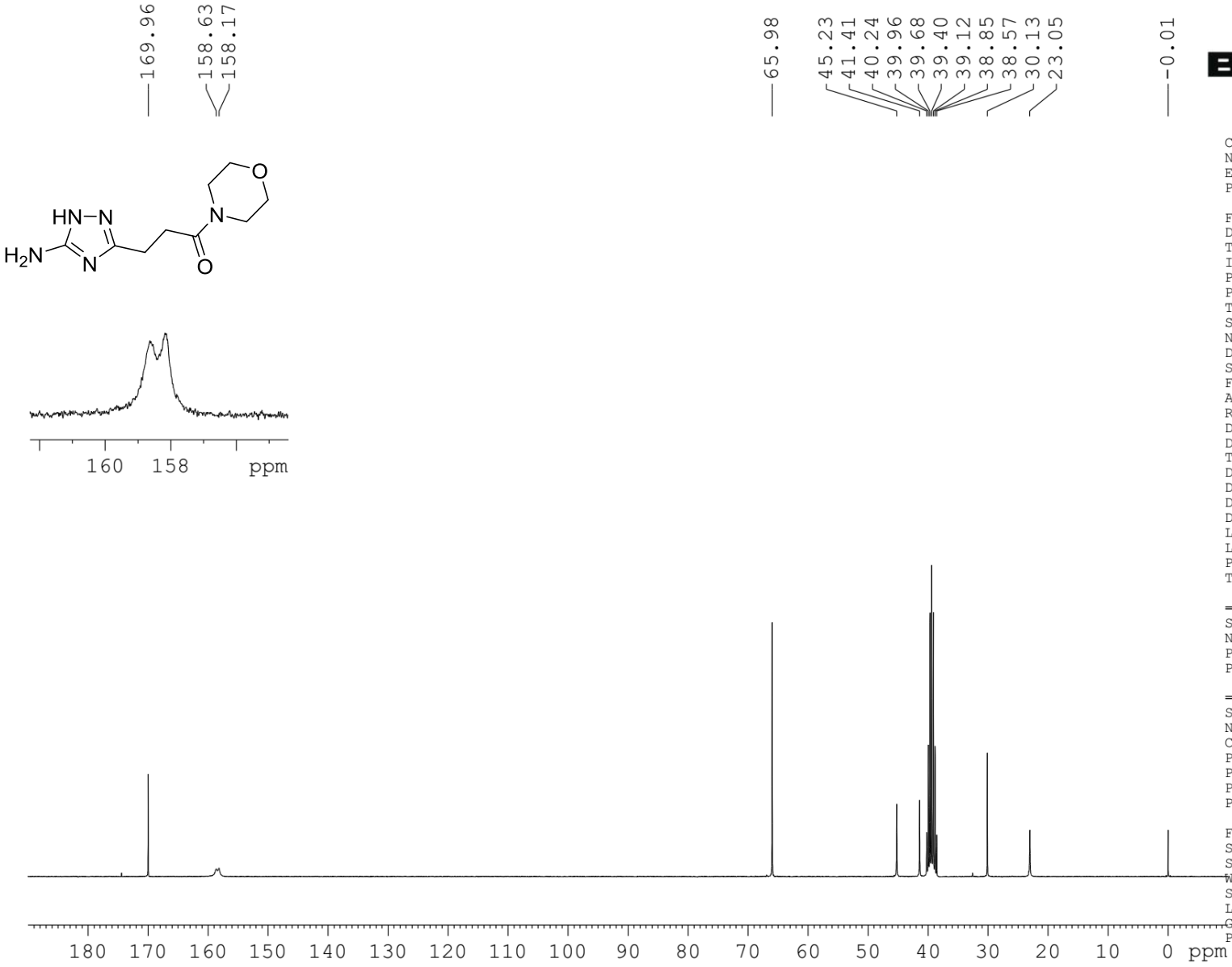

```
Current Data Parameters
NAME                  LY37
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20170707
Time                 17.54
INSTRUM       FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT               DMSO
NS                      16
DS                       2
SWH               6103.516 Hz
FIDRES            0.093132 Hz
AQ                5.3687091 sec
RG                  17.5543
DW                  81.920 usec
DE                    6.50 usec
TE                   300.2 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           300.1618536 MHz
NUC1                    1H
P1                   13.50 usec
PLW1            9.30000019 W

F2 - Processing parameters
SI                   65536
SF             300.1599984 MHz
WDW                     EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-1-morpholinopropan-1-one (5a)



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```
Current Data Parameters
NAME                  LY37
EXPNO                    2
PROCNO                   1

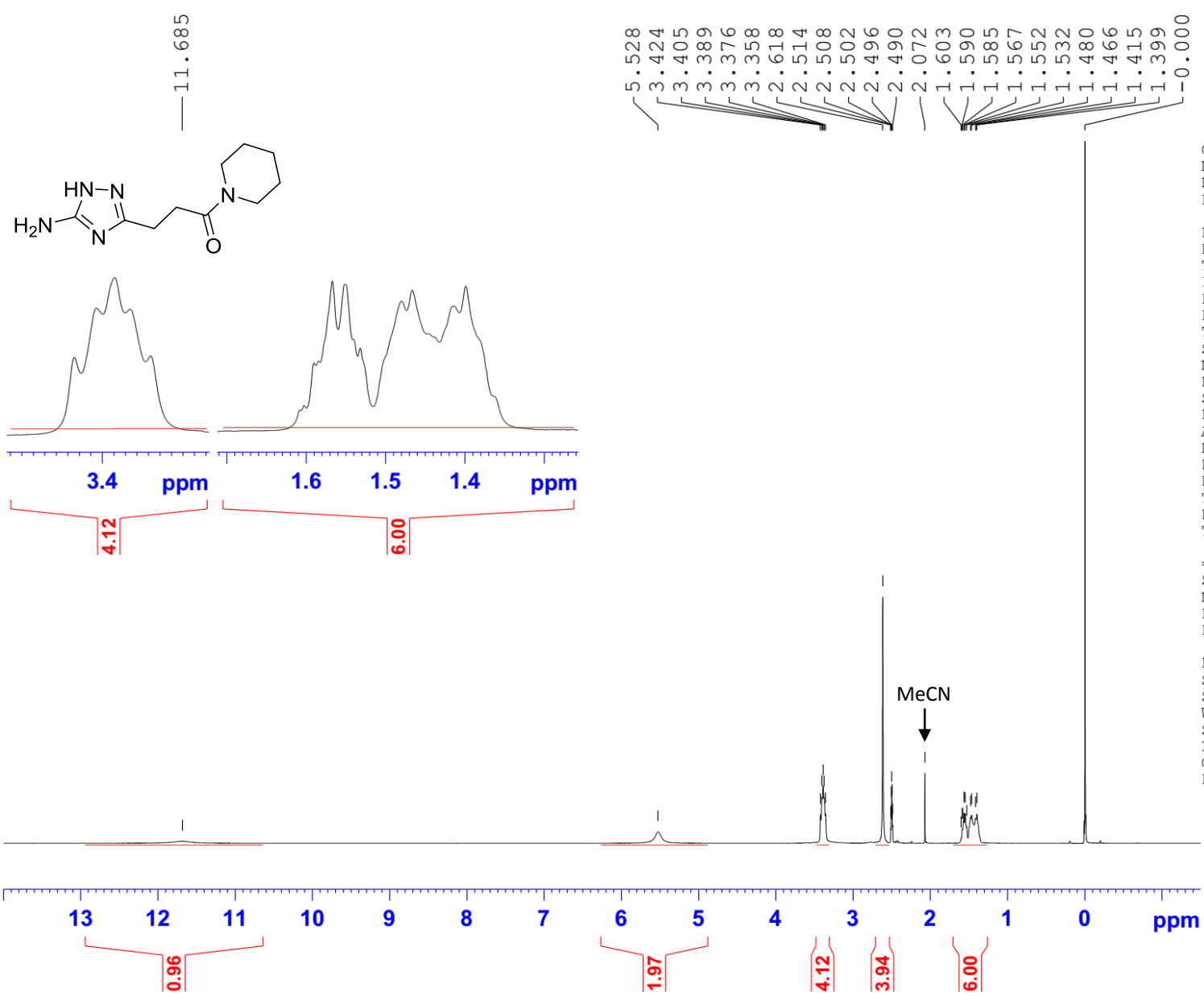
F2 - Acquisition Parameters
Date_              20170707
Time                 18.08
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT               DMSO
NS                   14336
DS                       4
SWH             24414.063 Hz
FIDRES           0.372529 Hz
AQ               1.3421773 sec
RG                 501.187
DW                  20.480 usec
DE                   6.50 usec
TE                  300.2 K
D1               2.00000000 sec
D11              0.03000000 sec
D31              0.00001500 sec
D40              0.00439029 sec
L4                      37
L5                      53
P32                 98.00 usec
TD0                     14

======== CHANNEL f1 ========
SFO1            75.4828392 MHz
NUC1                   13C
P1                  15.00 usec
PLW1           22.00000000 W

======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2               98.00 usec
PLW2            9.30000019 W
PLW12           0.29359001 W
PLW13           0.20359001 W

F2 - Processing parameters
SI                    32768
SF              75.4753336 MHz
WDW                      EM
SSB         0
LB                   1.00 Hz
GB          0
PC                   1.40
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-1-(piperidin-1-yl)propan-1-one (5b)



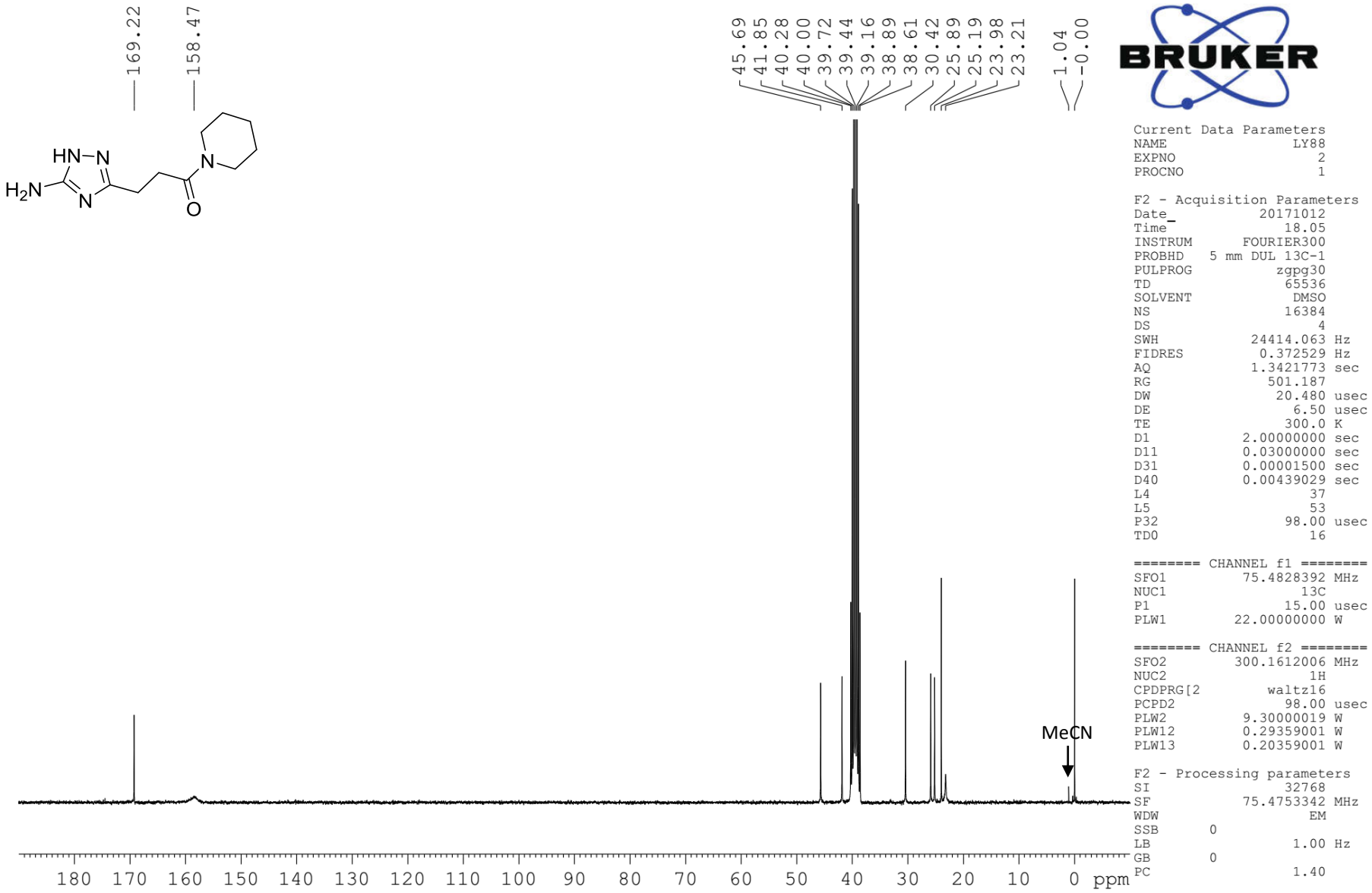

```
Current Data Parameters
NAME                  LY88
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20171011
Time                 16.14
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT               DMSO
NS                      16
DS                       2
SWH               6103.516 Hz
FIDRES             0.093132 Hz
AQ                5.3687091 sec
RG                   31.623
DW                  81.920 usec
DE                   6.50 usec
TE                  300.0 K
D1               1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           300.1618536 MHz
NUC1                     1H
P1                    13.50 usec
PLW1            9.30000019 W

F2 - Processing parameters
SI                   65536
SF             300.1600001 MHz
WDW                     EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-1-(piperidin-1-yl)propan-1-one (5b)



BRUKER

```
Current Data Parameters
NAME                  LY88
EXPNO                    2
PROCNO                   1

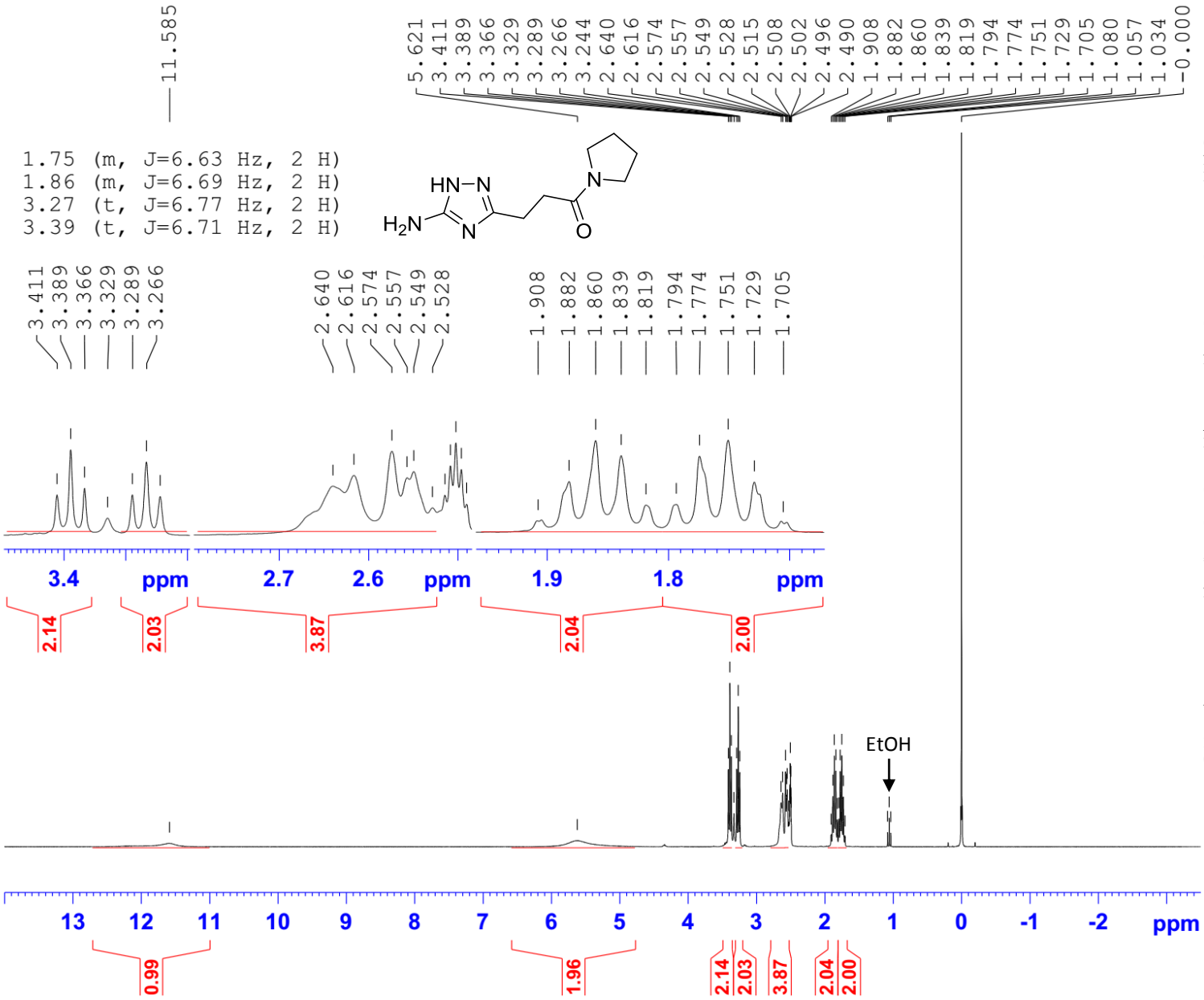
F2 - Acquisition Parameters
Date_              20171012
Time                 18.05
INSTRUM       FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG            zgpg30
TD                   65536
SOLVENT               DMSO
NS                   16384
DS                       4
SWH              24414.063 Hz
FIDRES               0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                   20.480 usec
DE                    6.50 usec
TE                   300.0 K
D1             2.00000000 sec
D11            0.03000000 sec
D31            0.00001500 sec
D40            0.00439029 sec
L4                      37
L5                      53
P32                  98.00 usec
TD0                     16

======== CHANNEL f1 ========
SFO1            75.4828392 MHz
NUC1                   13C
P1                   15.00 usec
PLW1           22.00000000 W

======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2                98.00 usec
PLW2            9.30000019 W
PLW12           0.29359001 W
PLW13           0.20359001 W

F2 - Processing parameters
SI                    32768
SF              75.4753342 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-1-(pyrrolidin-1-yl)propan-1-one (5c)



BRUKER

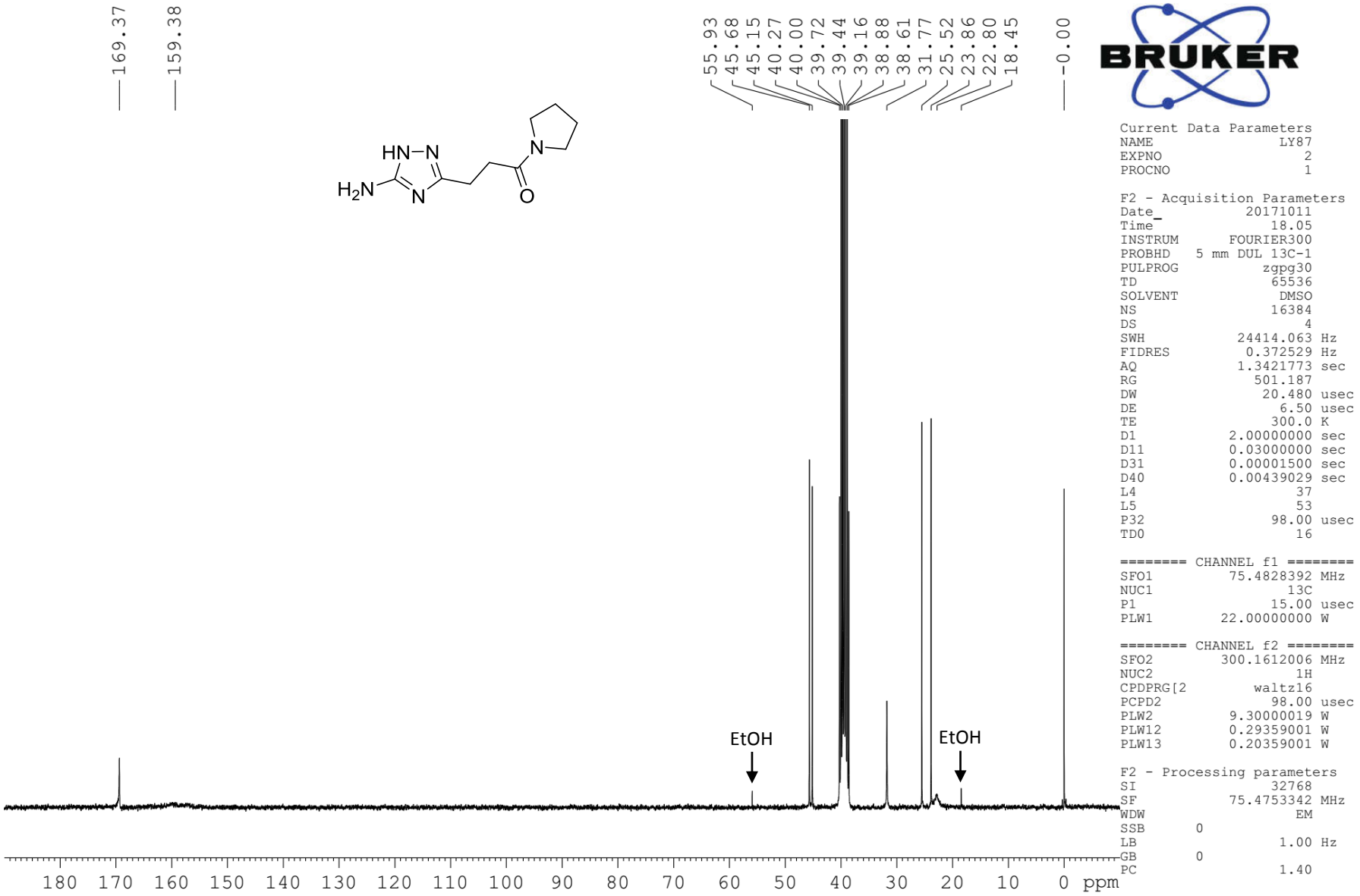
```
Current Data Parameters
NAME                  LY87
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20171011
Time                 16.10
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT               DMSO
NS                      16
DS                       2
SWH               6103.516 Hz
FIDRES           0.093132 Hz
AQ               5.3687091 sec
RG                    31.623
DW                   81.920 usec
DE                    6.50 usec
TE                   299.9 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          300.1618536 MHz
NUC1                    1H
P1                   13.50 usec
PLW1           9.30000019 W

F2 - Processing parameters
SI                   65536
SF            300.1600000 MHz
WDW                     EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-1-(pyrrolidin-1-yl)propan-1-one (5c)



BRUKER

```
Current Data Parameters
NAME                  LY87
EXPNO                    2
PROCNO                   1

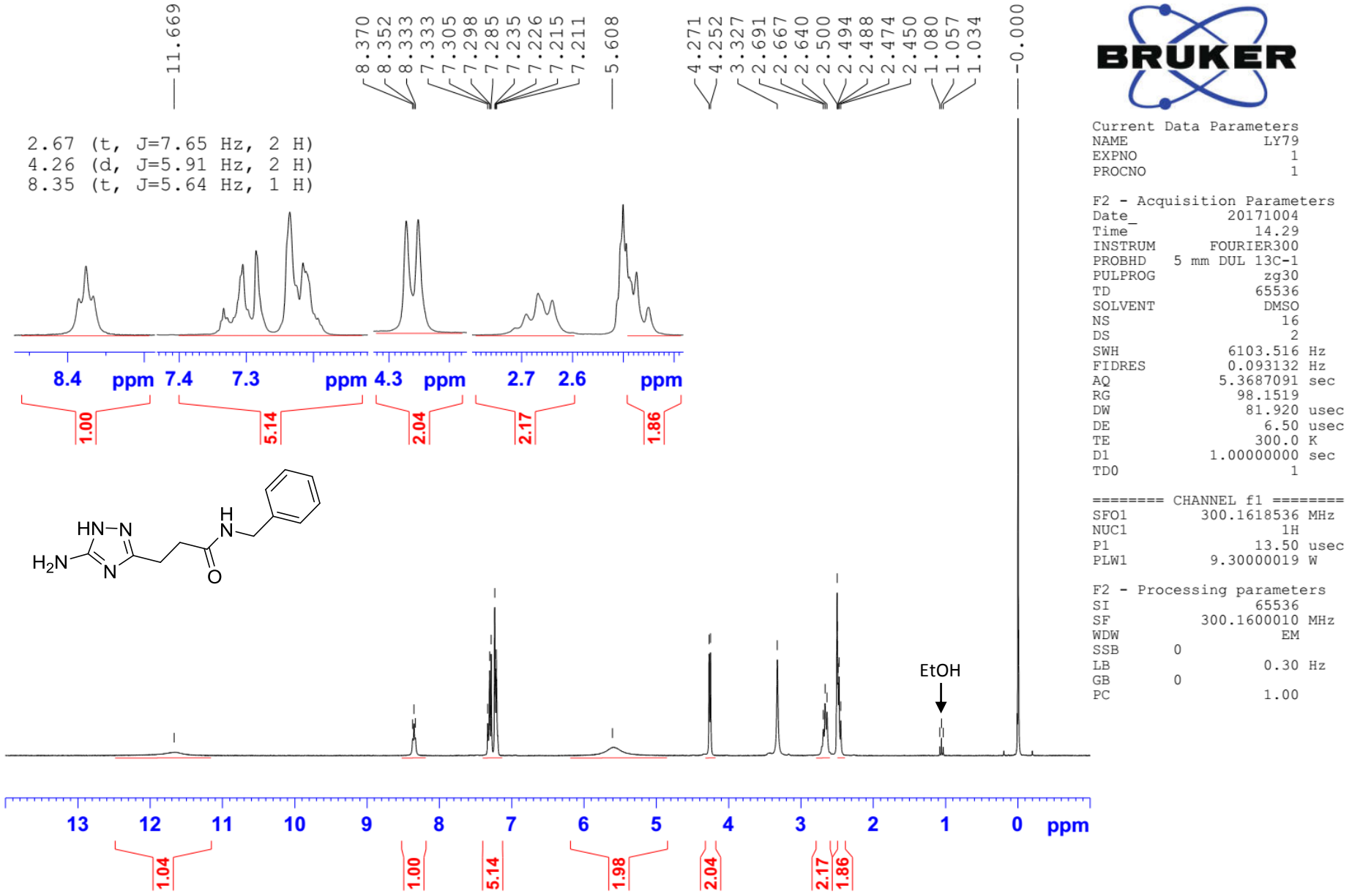
F2 - Acquisition Parameters
Date_              20171011
Time                 18.05
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG            zgpg30
TD                  65536
SOLVENT              DMSO
NS                   16384
DS                       4
SWH             24414.063 Hz
FIDRES           0.372529 Hz
AQ               1.3421773 sec
RG                 501.187
DW                  20.480 usec
DE                   6.50 usec
TE                  300.0 K
D1               2.00000000 sec
D11              0.03000000 sec
D31              0.00001500 sec
D40              0.00439029 sec
L4                      37
L5                      53
P32                  98.00 usec
TD0                     16

======== CHANNEL f1 ========
SFO1            75.4828392 MHz
NUC1                   13C
P1                   15.00 usec
PLW1           22.00000000 W

======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2                98.00 usec
PLW2            9.30000019 W
PLW12           0.29359001 W
PLW13           0.20359001 W

F2 - Processing parameters
SI                    32768
SF              75.4753342 MHz
WDW                      EM
SSB         0
LB                    1.00 Hz
GB          0
PC                    1.40
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(4-benzyl)propanamide (5d)



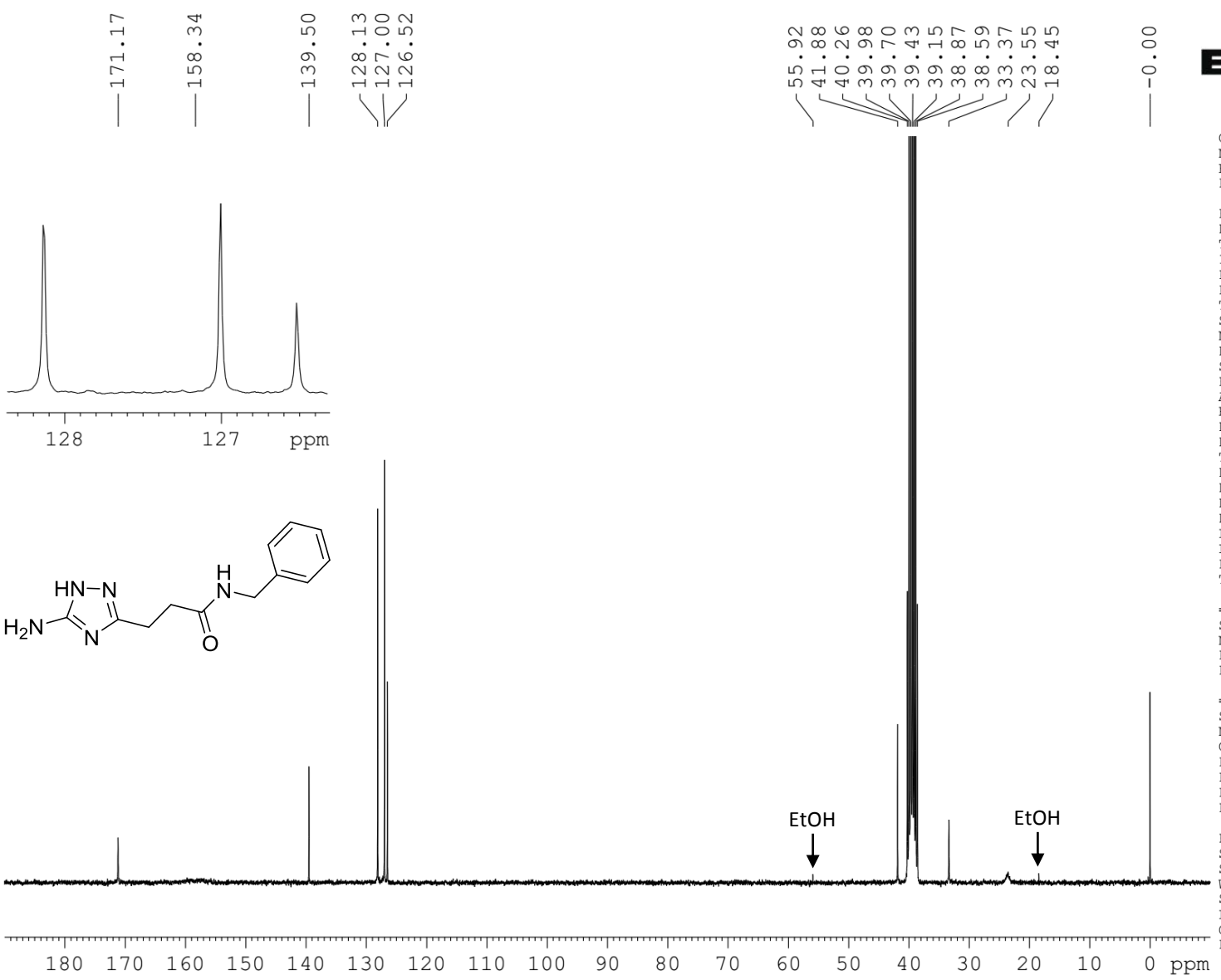

```
Current Data Parameters
NAME                  LY79
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20171004
Time                 14.29
INSTRUM       FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT               DMSO
NS                      16
DS                       2
SWH               6103.516 Hz
FIDRES           0.093132 Hz
AQ                5.3687091 sec
RG                  98.1519
DW                  81.920 usec
DE                   6.50 usec
TE                  300.0 K
D1               1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           300.1618536 MHz
NUC1                    1H
P1                   13.50 usec
PLW1            9.30000019 W

F2 - Processing parameters
SI                   65536
SF             300.1600010 MHz
WDW                     EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(4-benzyl)propanamide (5d)



BRUKER

```
Current Data Parameters
NAME                  LY79
EXPNO                    3
PROCNO                   1

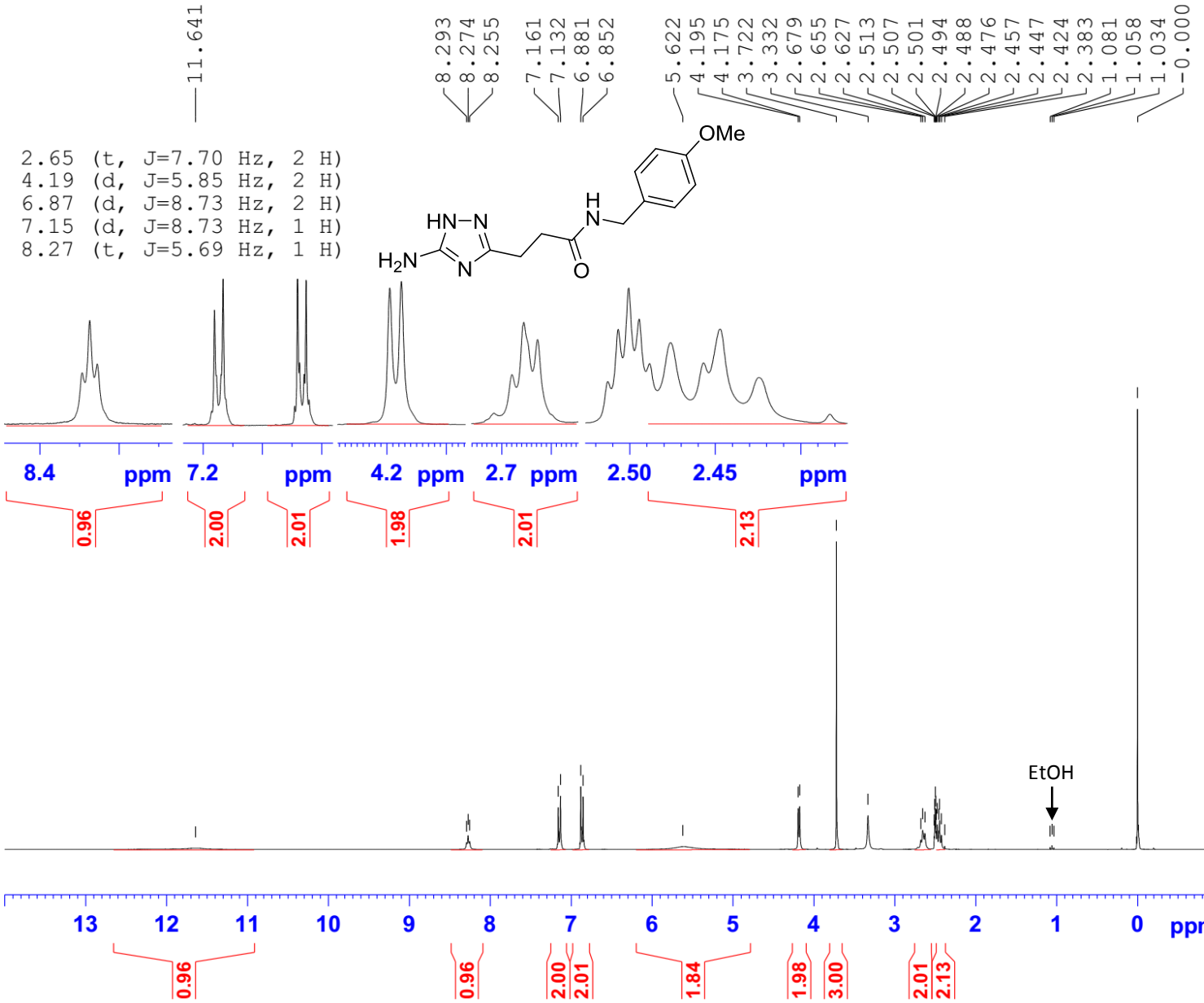
F2 - Acquisition Parameters
Date_              20171009
Time                 18.05
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG              zgpg30
TD                    65536
SOLVENT                DMSO
NS                    16384
DS                        4
SWH              24414.063 Hz
FIDRES            0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                   20.480 usec
DE                    6.50 usec
TE                   300.0 K
D1             2.00000000 sec
D11            0.03000000 sec
D31            0.00001500 sec
D40            0.00439029 sec
L4                       37
L5                       53
P32                   98.00 usec
TD0                      16

======== CHANNEL f1 ========
SFO1           75.4828392 MHz
NUC1                   13C
P1                    15.00 usec
PLW1          22.00000000 W

======== CHANNEL f2 ========
SFO2          300.1612006 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2                 98.00 usec
PLW2           9.30000019 W
PLW12          0.29359001 W
PLW13          0.20359001 W

F2 - Processing parameters
SI                    32768
SF             75.4753350 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(4-methoxybenzyl)propanamide (5e)



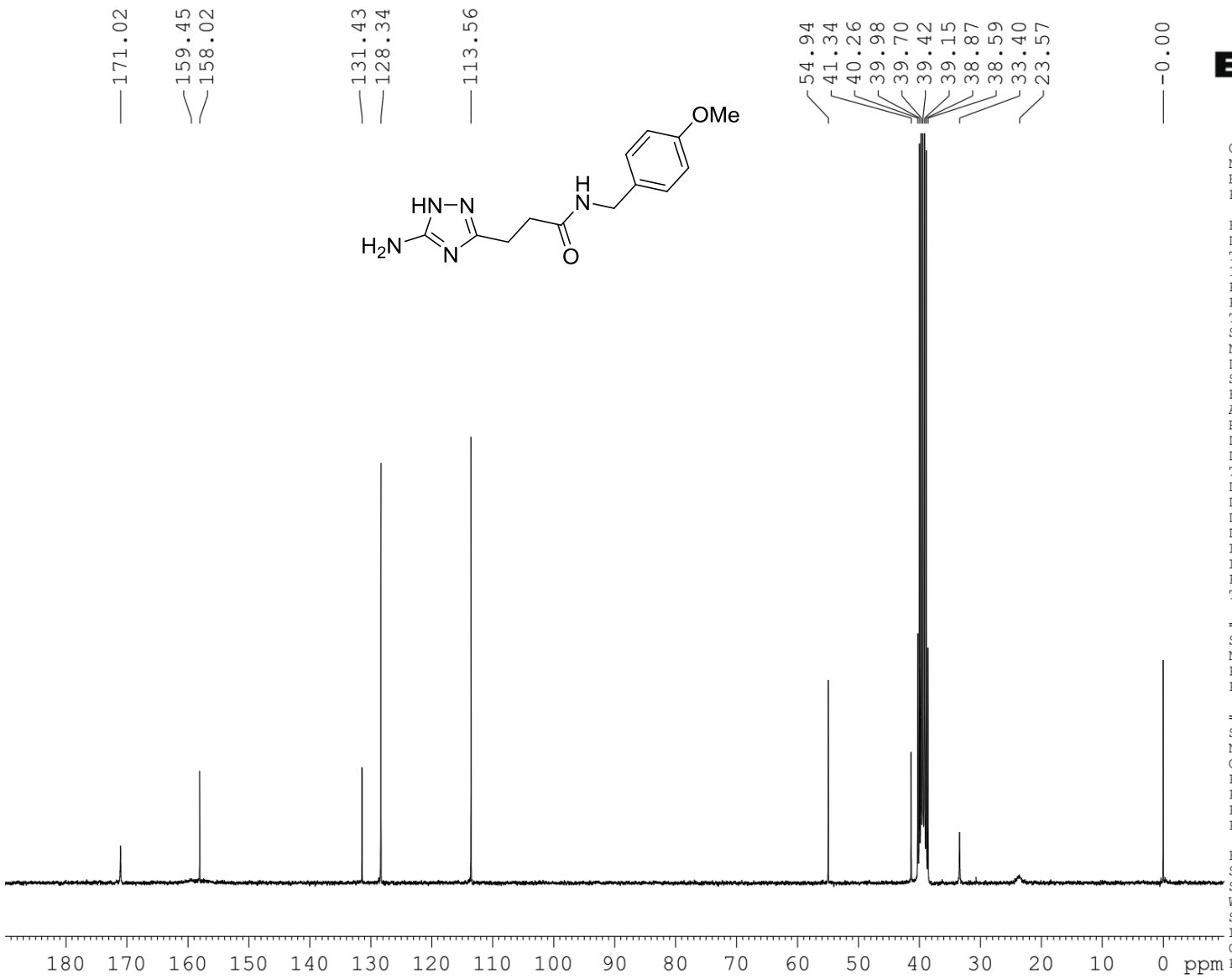

```
Current Data Parameters
NAME                  LY80
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20171004
Time                 14.34
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT               DMSO
NS                      16
DS                       2
SWH               6103.516 Hz
FIDRES            0.093132 Hz
AQ                5.3687091 sec
RG                   76.6739
DW                   81.920 usec
DE                    6.50 usec
TE                   300.1 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           300.1618536 MHz
NUC1                   1H
P1                   13.50 usec
PLW1            9.30000019 W

F2 - Processing parameters
SI                   65536
SF             300.1600006 MHz
WDW                    EM
SSB         0
LB                    0.30 Hz
GB          0
PC                    1.00
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(4-methoxybenzyl)propanamide (5e)




```
Current Data Parameters
NAME                  LY80
EXPNO                    3
PROCNO                   1

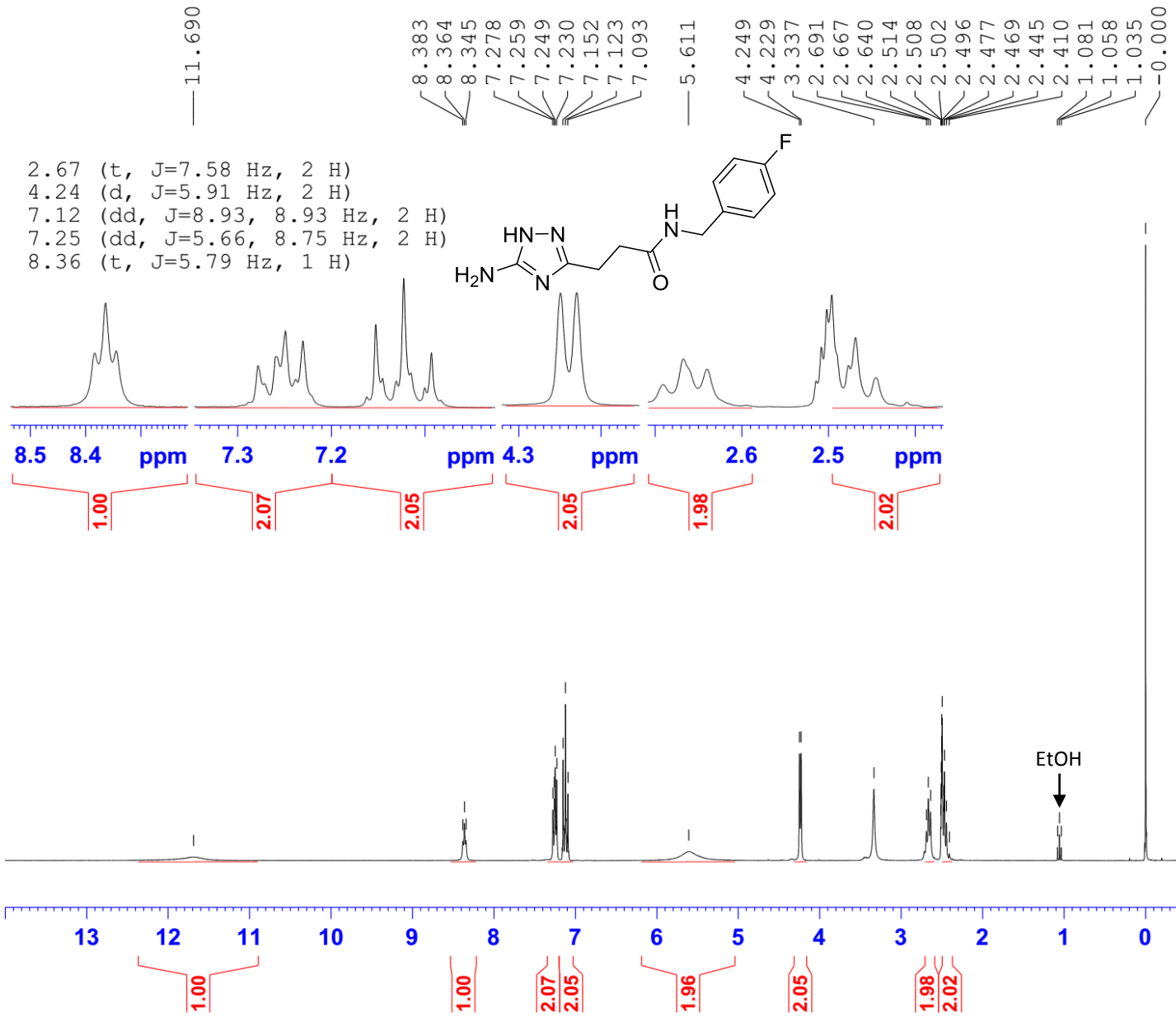
F2 - Acquisition Parameters
Date_              20171010
Time                 18.09
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG            zgpg30
TD                  65536
SOLVENT               DMSO
NS                  16384
DS                      4
SWH             24414.063 Hz
FIDRES              0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                   20.480 usec
DE                    6.50 usec
TE                   300.0 K
D1             2.00000000 sec
D11            0.03000000 sec
D31            0.00001500 sec
D40            0.00439029 sec
L4                      37
L5                      53
P32                  98.00 usec
TD0                     16

======== CHANNEL f1 ========
SFO1           75.4828392 MHz
NUC1                   13C
P1                   15.00 usec
PLW1          22.00000000 W

======== CHANNEL f2 ========
SFO2          300.1612006 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2                98.00 usec
PLW2           9.30000019 W
PLW12          0.29359001 W
PLW13          0.20359001 W

F2 - Processing parameters
SI                    32768
SF             75.4753350 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(4-fluorobenzyl)propanamide (5f)



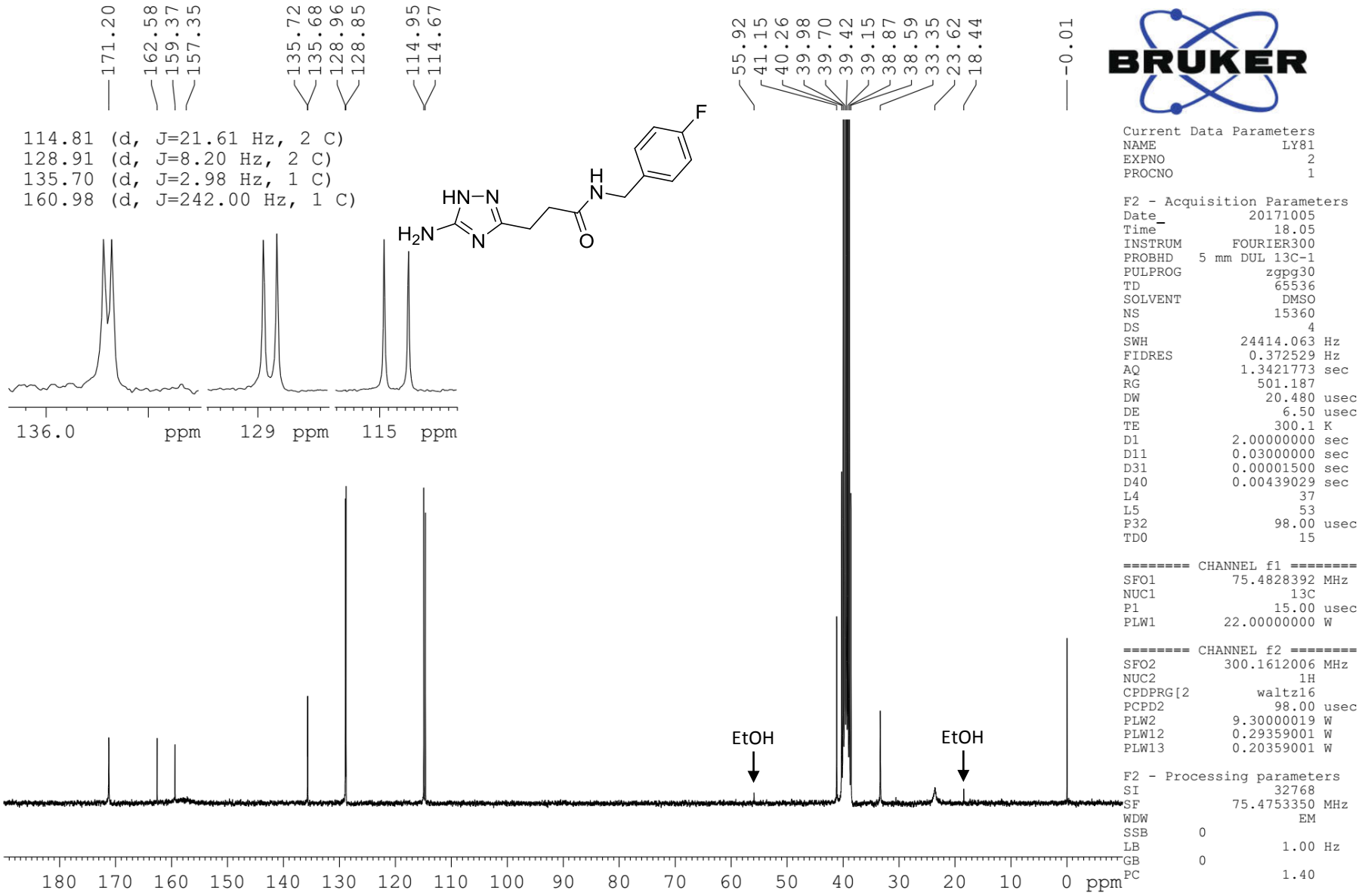

```
Current Data Parameters
NAME                  LY81
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20171005
Time                 16.17
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT               DMSO
NS                      16
DS                       2
SWH               6103.516 Hz
FIDRES           0.093132 Hz
AQ                5.3687091 sec
RG                  89.3912
DW                  81.920 usec
DE                   6.50 usec
TE                  300.1 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           300.1618536 MHz
NUC1                   1H
P1                  13.50 usec
PLW1           9.30000019 W

F2 - Processing parameters
SI                   65536
SF             300.1600001 MHz
WDW                    EM
SSB         0
LB                   0.30 Hz
GB          0
PC                   1.00
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(4-fluorobenzyl)propanamide (5f)



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Current Data Parameters
NAME LY81
EXPNO 2
PROCNO 1

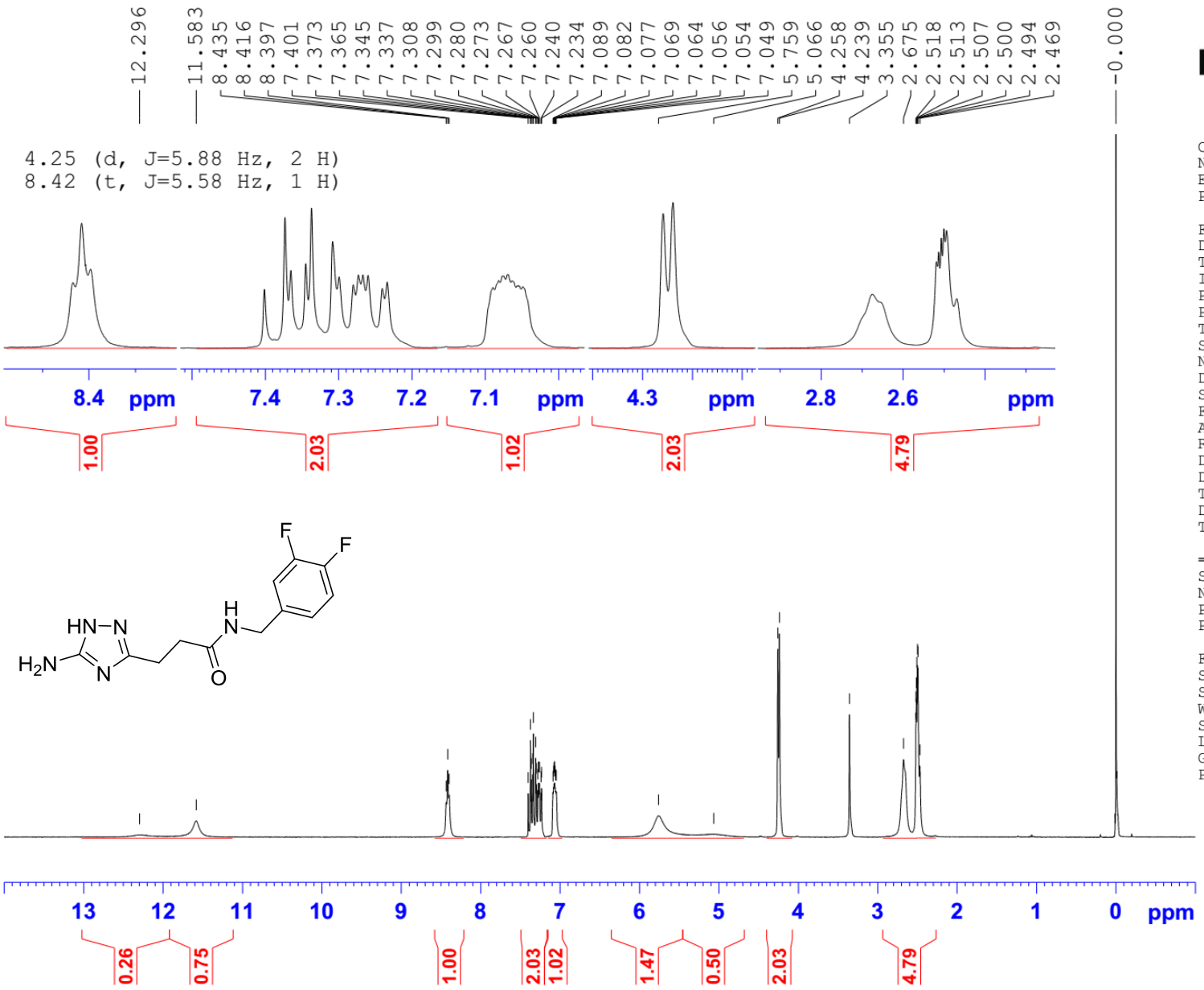
F2 - Acquisition Parameters
Date_ 20171005
Time 18.05
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 15360
DS 4
SWH 24414.063 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 501.187
DW 20.480 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
D11 0.03000000 sec
D31 0.00001500 sec
D40 0.00439029 sec
L4 37
L5 53
P32 98.00 usec
TD0 15

======== CHANNEL f1 ========
SFO1 75.4828392 MHz
NUC1 13C
P1 15.00 usec
PLW1 22.00000000 W

======== CHANNEL f2 ========
SFO2 300.1612006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 98.00 usec
PLW2 9.30000019 W
PLW12 0.29359001 W
PLW13 0.20359001 W

F2 - Processing parameters
SI 32768
SF 75.4753350 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(3,4-difluorobenzyl)propanamide (5g)



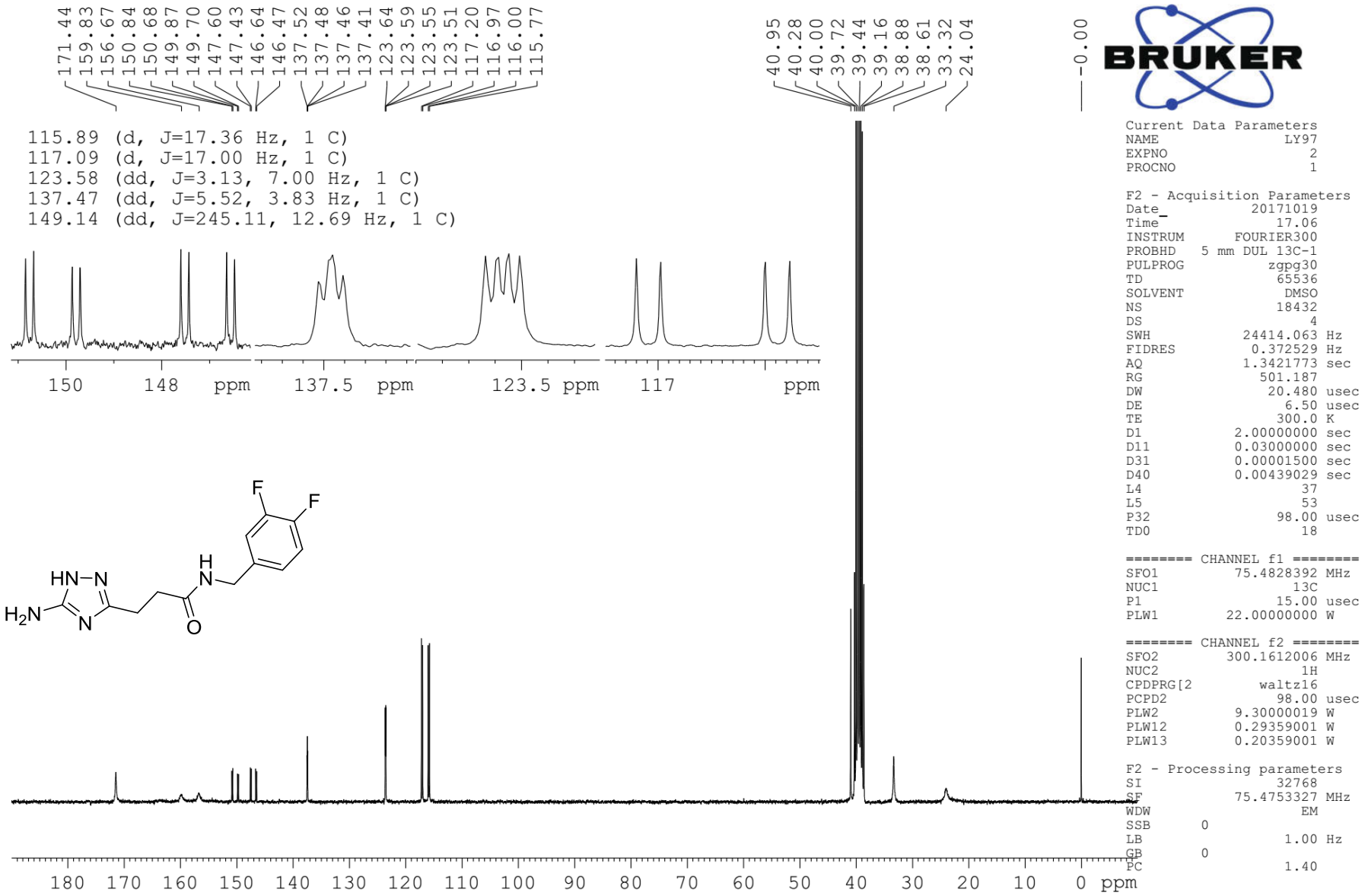

```
Current Data Parameters
NAME                  LY97
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20171019
Time                 15.36
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT               DMSO
NS                      16
DS                       2
SWH               6103.516 Hz
FIDRES               0.093132 Hz
AQ                5.3687091 sec
RG                    63.133
DW                   81.920 usec
DE                    6.50 usec
TE                   300.0 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           300.1618536 MHz
NUC1                    1H
P1                   13.50 usec
PLW1            9.30000019 W

F2 - Processing parameters
SI                   65536
SF             300.1599990 MHz
WDW                     EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(3,4-difluorobenzyl)propanamide (5g)



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```
Current Data Parameters
NAME                  LY97
EXPNO                    2
PROCNO                   1

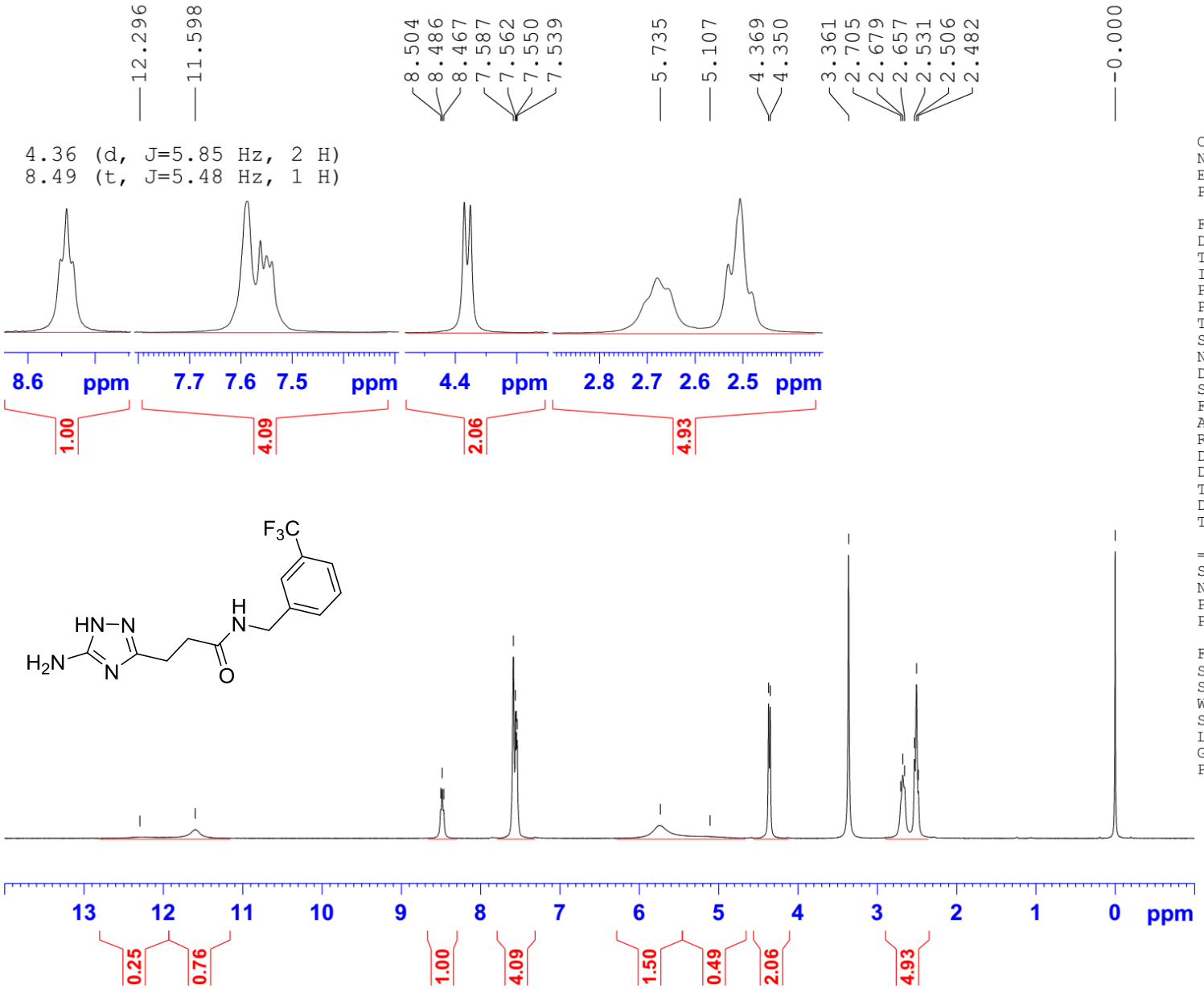
F2 - Acquisition Parameters
Date_              20171019
Time                 17.06
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                   18432
DS                       4
SWH              24414.063 Hz
FIDRES           0.372529 Hz
AQ               1.3421773 sec
RG                 501.187
DW                  20.480 usec
DE                   6.50 usec
TE                  300.0 K
D1             2.00000000 sec
D11            0.03000000 sec
D31            0.00001500 sec
D40            0.00439029 sec
L4                      37
L5                      53
P32                  98.00 usec
TD0                     18

======== CHANNEL f1 ========
SFO1           75.4828392 MHz
NUC1                   13C
P1                   15.00 usec
PLW1          22.00000000 W

======== CHANNEL f2 ========
SFO2          300.1612006 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2                98.00 usec
PLW2           9.30000019 W
PLW12          0.29359001 W
PLW13          0.20359001 W

F2 - Processing parameters
SI                    32768
SF             75.4753327 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(3-trifluoromethylbenzyl)propanamide (5h)



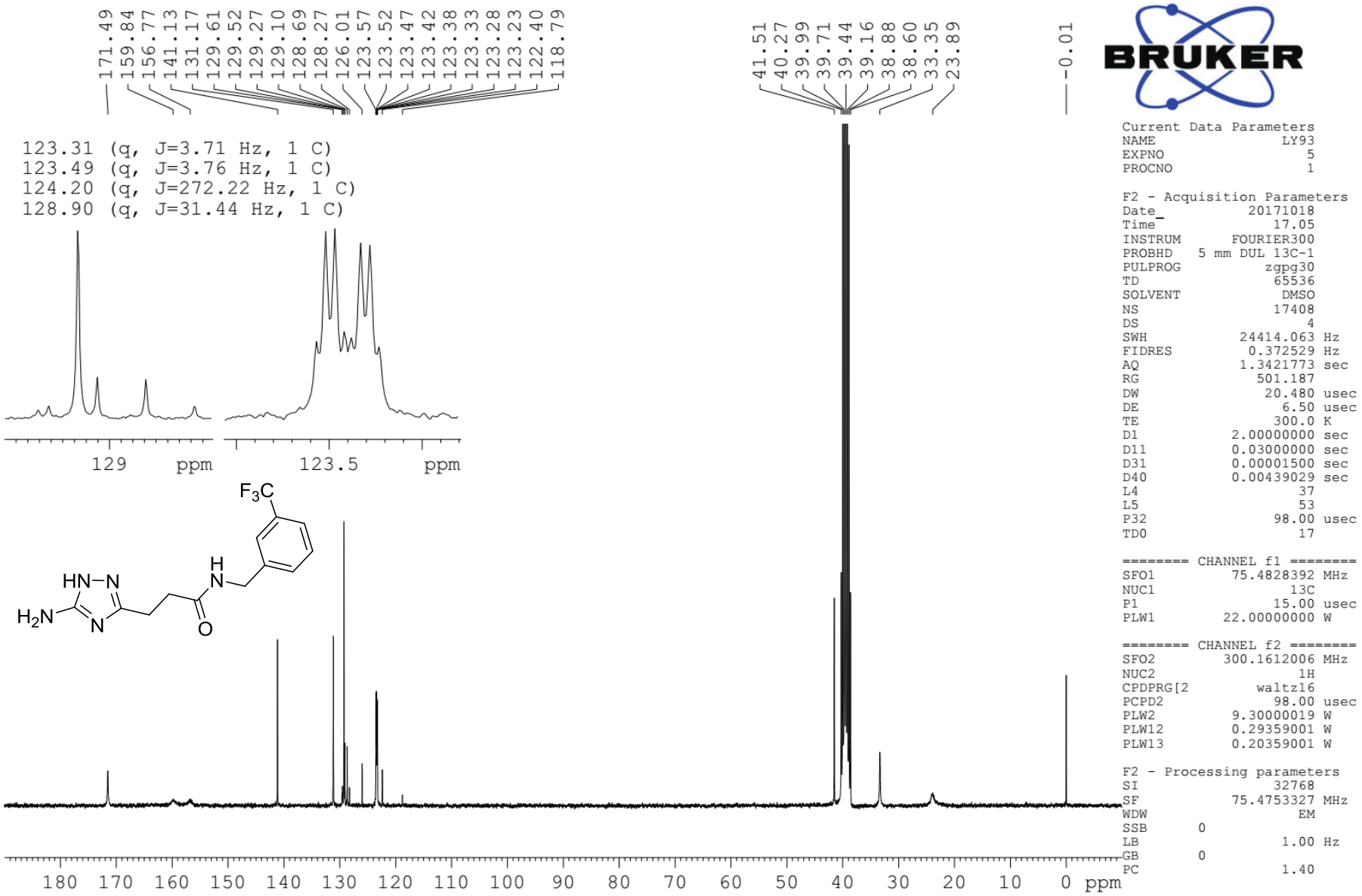

```
Current Data Parameters
NAME                  LY93
EXPNO                    4
PROCNO                   1

F2 - Acquisition Parameters
Date_              20171018
Time                 12.12
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT               DMSO
NS                      16
DS                       2
SWH               6103.516 Hz
FIDRES               0.093132 Hz
AQ                5.3687091 sec
RG                  58.2496
DW                  81.920 usec
DE                   6.50 usec
TE                  300.0 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           300.1618536 MHz
NUC1                    1H
P1                   13.50 usec
PLW1            9.30000019 W

F2 - Processing parameters
SI                   65536
SF             300.1599986 MHz
WDW                     EM
SSB          0
LB                   0.30 Hz
GB           0
PC                   1.00
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(3-trifluoromethylbenzyl)propanamide (5h)



BRUKER

Current Data Parameters
NAME LY93
EXPNO 5
PROCNO 1

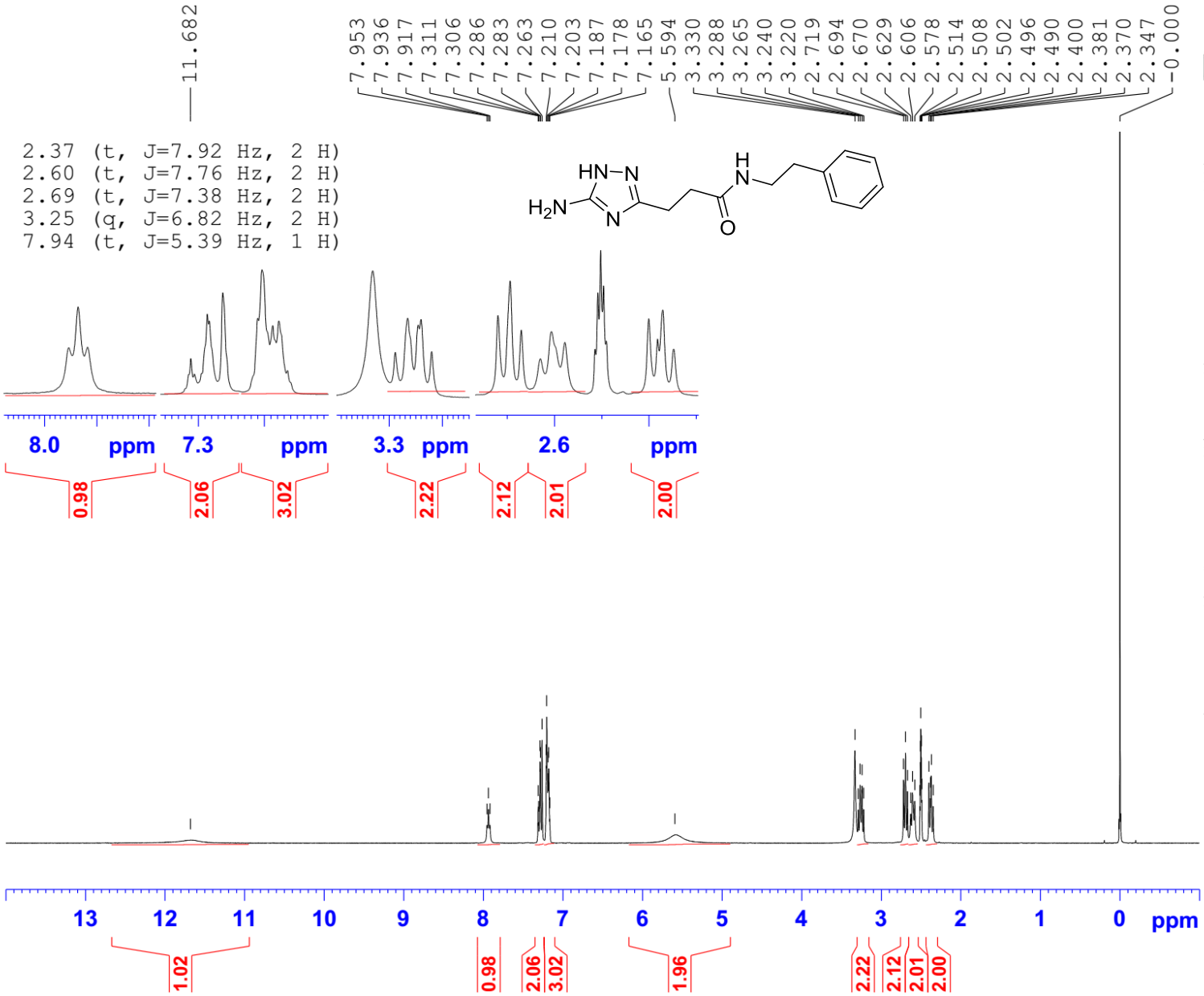
F2 - Acquisition Parameters
Date_ 20171018
Time 17.05
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 17408
DS 4
SWH 24414.063 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 501.187
DW 20.480 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D31 0.00001500 sec
D40 0.00439029 sec
L4 37
L5 53
P32 98.00 usec
TD0 17

======== CHANNEL f1 ========
SFO1 75.4828392 MHz
NUC1 13C
P1 15.00 usec
PLW1 22.00000000 W

======== CHANNEL f2 ========
SFO2 300.1612006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 98.00 usec
PLW2 9.30000019 W
PLW12 0.29359001 W
PLW13 0.20359001 W

F2 - Processing parameters
SI 32768
SF 75.4753327 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(phenylethyl)propanamide (5i)



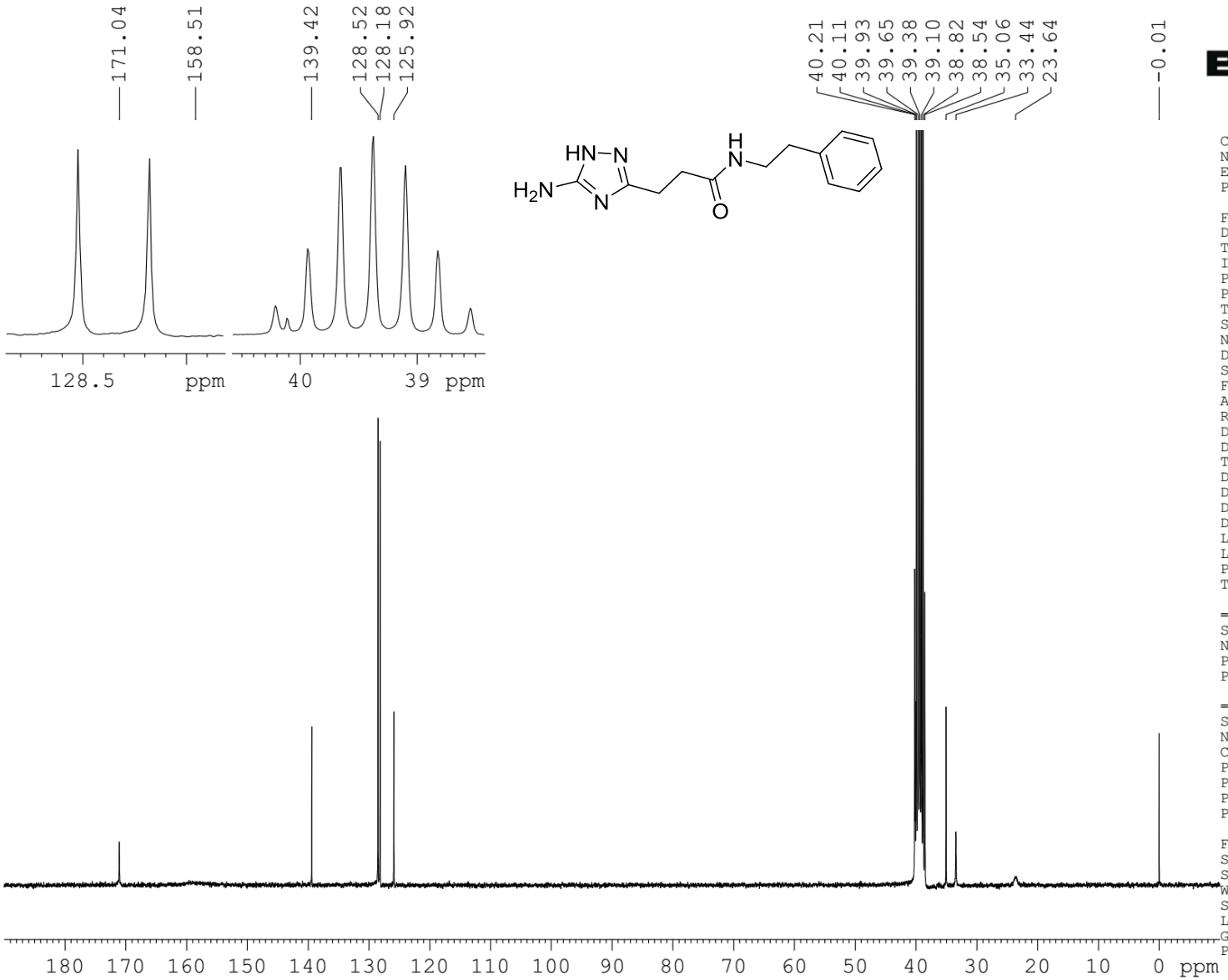

```
Current Data Parameters
NAME                  LY82
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20171005
Time                 16.22
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT               DMSO
NS                      16
DS                       2
SWH               6103.516 Hz
FIDRES               0.093132 Hz
AQ                5.3687091 sec
RG                  84.3829
DW                  81.920 usec
DE                   6.50 usec
TE                  300.1 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           300.1618536 MHz
NUC1                    1H
P1                   13.50 usec
PLW1            9.30000019 W

F2 - Processing parameters
SI                   65536
SF             300.1600003 MHz
WDW                     EM
SSB          0
LB                   0.30 Hz
GB           0
PC                   1.00
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(phenylethyl)propanamide (5i)



BRUKER

```
Current Data Parameters
NAME                  LY82
EXPNO                    2
PROCNO                   1

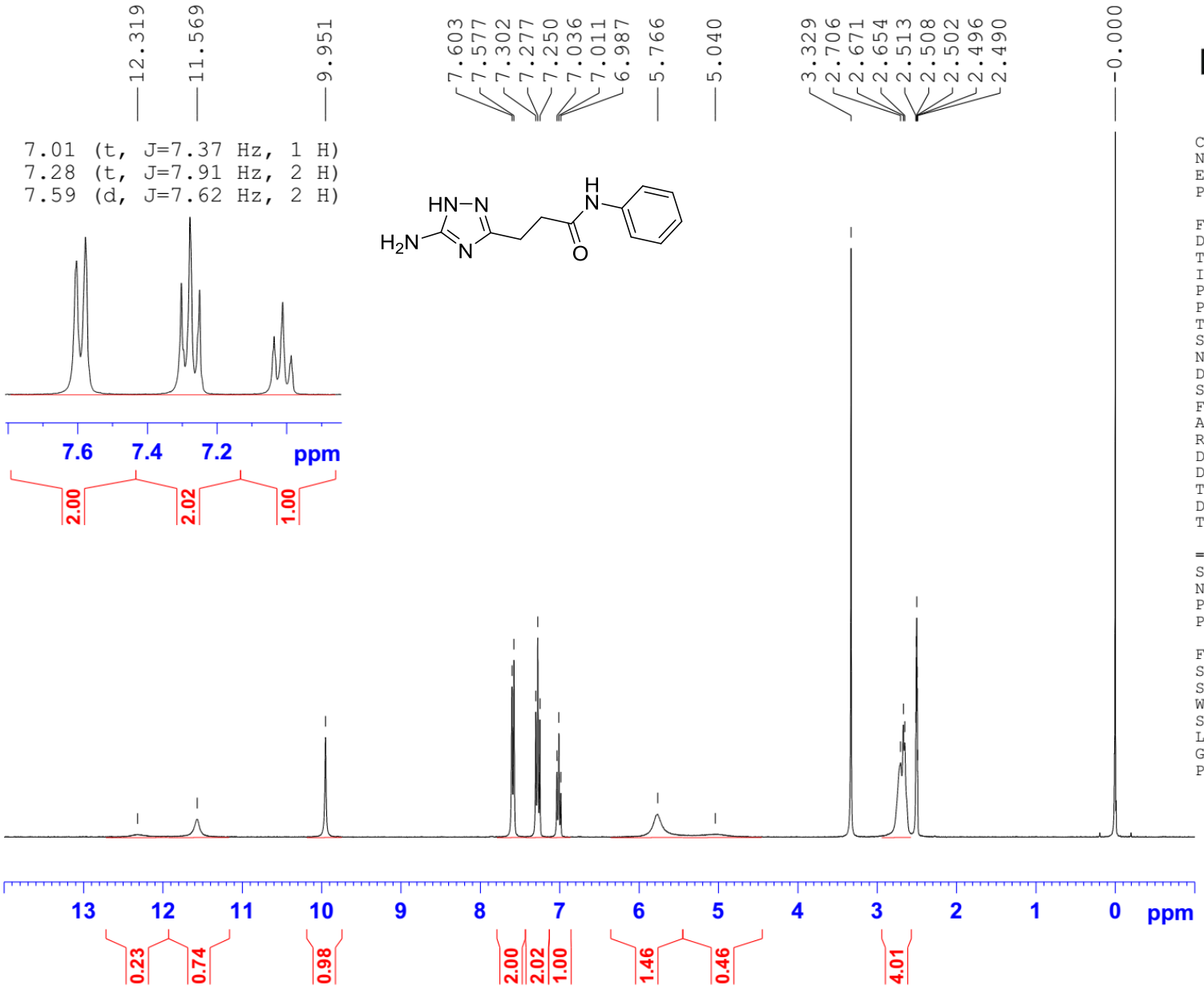
F2 - Acquisition Parameters
Date_              20171007
Time                 19.28
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                   15360
DS                       4
SWH              24414.063 Hz
FIDRES            0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                   20.480 usec
DE                    6.50 usec
TE                   295.9 K
D1                2.00000000 sec
D11               0.03000000 sec
D31               0.00001500 sec
D40               0.00439029 sec
L4                       37
L5                       53
P32                   98.00 usec
TD0                      15

======== CHANNEL f1 ========
SFO1             75.4828392 MHz
NUC1                    13C
P1                    15.00 usec
PLW1           22.00000000 W

======== CHANNEL f2 ========
SFO2            300.1612006 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                 98.00 usec
PLW2              9.30000019 W
PLW12             0.29359001 W
PLW13             0.20359001 W

F2 - Processing parameters
SI                      32768
SF               75.4753357 MHz
WDW                        EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(phenyl)propanamide (5j)



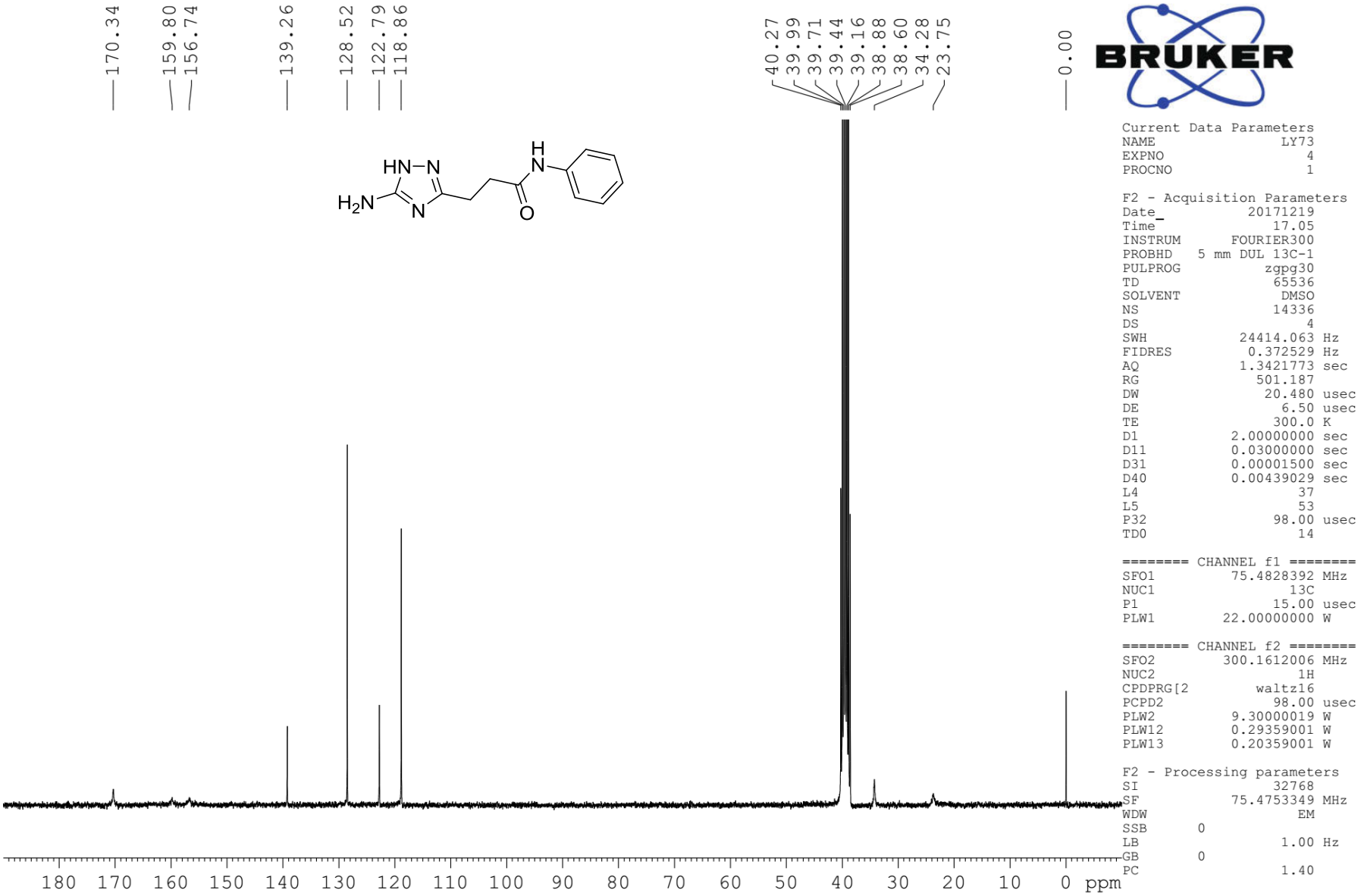

```
Current Data Parameters
NAME                  LY73
EXPNO                    3
PROCNO                   1

F2 - Acquisition Parameters
Date_              20171219
Time                 13.25
INSTRUM       FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                     16
DS                      2
SWH               6103.516 Hz
FIDRES            0.093132 Hz
AQ                5.3687091 sec
RG                  115.753
DW                   81.920 usec
DE                    6.50 usec
TE                   300.1 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1          300.1618536 MHz
NUC1                    1H
P1                   13.50 usec
PLW1           9.30000019 W

F2 - Processing parameters
SI                    65536
SF            300.1600000 MHz
WDW                     EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(phenyl)propanamide (5j)



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```
Current Data Parameters
NAME                  LY73
EXPNO                    4
PROCNO                   1

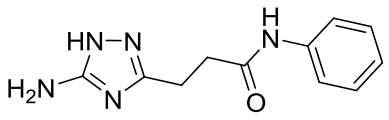
F2 - Acquisition Parameters
Date_              20171219
Time                 17.05
INSTRUM       FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG            zgpg30
TD                  65536
SOLVENT               DMSO
NS                  14336
DS                      4
SWH             24414.063 Hz
FIDRES           0.372529 Hz
AQ               1.3421773 sec
RG                501.187
DW                 20.480 usec
DE                  6.50 usec
TE                 300.0 K
D1              2.00000000 sec
D11             0.03000000 sec
D31             0.00001500 sec
D40             0.00439029 sec
L4                     37
L5                     53
P32                98.00 usec
TD0                    14

======== CHANNEL f1 ========
SFO1            75.4828392 MHz
NUC1                   13C
P1                  15.00 usec
PLW1          22.00000000 W

======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2               98.00 usec
PLW2           9.30000019 W
PLW12          0.29359001 W
PLW13          0.20359001 W

F2 - Processing parameters
SI                  32768
SF             75.4753349 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(phenyl)propanamide (5j)




```
Current Data Parameters
NAME                  LY73
EXPNO                    6
PROCNO                   1

F2 - Acquisition Parameters
Date_              20171231
Time                 19.46
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG     hmbcgplpndqf
TD                    2048
SOLVENT               DMSO
NS                     250
DS                      16
SWH              6103.516 Hz
FIDRES           2.980232 Hz
AQ               0.1677722 sec
RG                501.187
DW                 81.920 usec
DE                  6.50 usec
TE                299.9 K
CNST2         145.0000000
CNST13         10.0000000
D0             0.00000300 sec
D1             1.42610800 sec
D2             0.00344828 sec
D6             0.05000000 sec
D16            0.00020000 sec
D31            0.00001350 sec
D32            0.00002700 sec
D33            0.00001200 sec
D36            0.00100000 sec
D38            0.00002980 sec
IN0            0.00002980 sec

======== CHANNEL f1 ========
SFO1          300.1618659 MHz
NUC1                  1H
P1                 13.50 usec
P2                 27.00 usec
PLW1           9.30000019 W

======== CHANNEL f2 ========
SFO2           75.4828272 MHz
NUC2                 13C
P3                 12.00 usec
PLW2          22.00000000 W

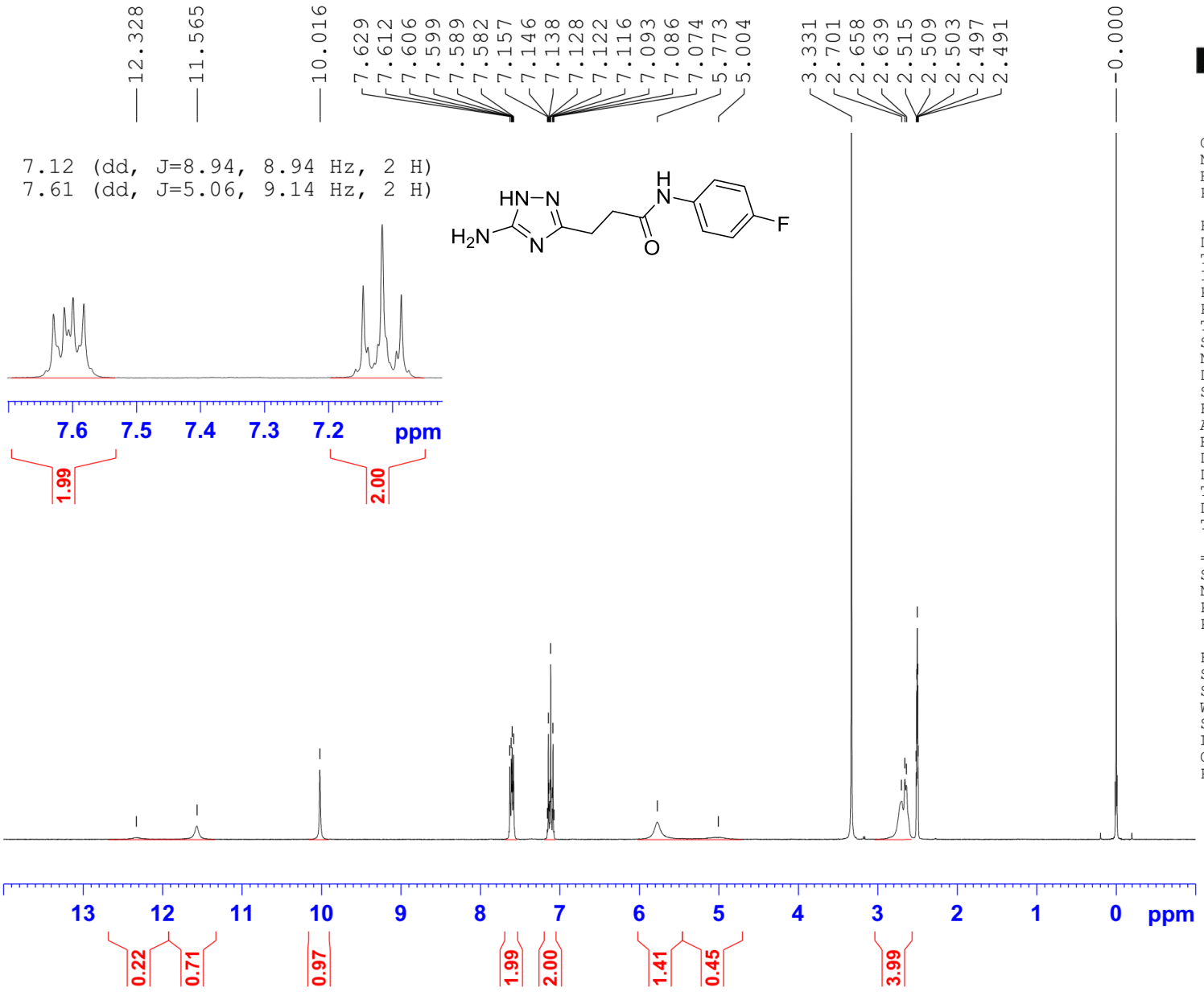
====== GRADIENT CHANNEL =====
GPNAM[1]           RECT.1
GPNAM[2]           RECT.1
GPNAM[3]           RECT.1
GPZ1                50.00 %
GPZ2                30.00 %
GPZ3                40.10 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                    128
SFO1            75.48283 MHz
FIDRES         131.082214 Hz
SW               222.283 ppm
FnMODE                QF

F2 - Processing parameters
SI                    2048
SF            300.1600018 MHz
WDW                   SINE
SSB         0
LB          0 Hz
GB          0
PC                   1.40

F1 - Processing parameters
SI                    1024
MC2                     QF
SF             75.4753377 MHz
WDW                   SINE
SSB         0
LB          0 Hz
GB          0
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(4-fluorophenyl)propanamide (5k)



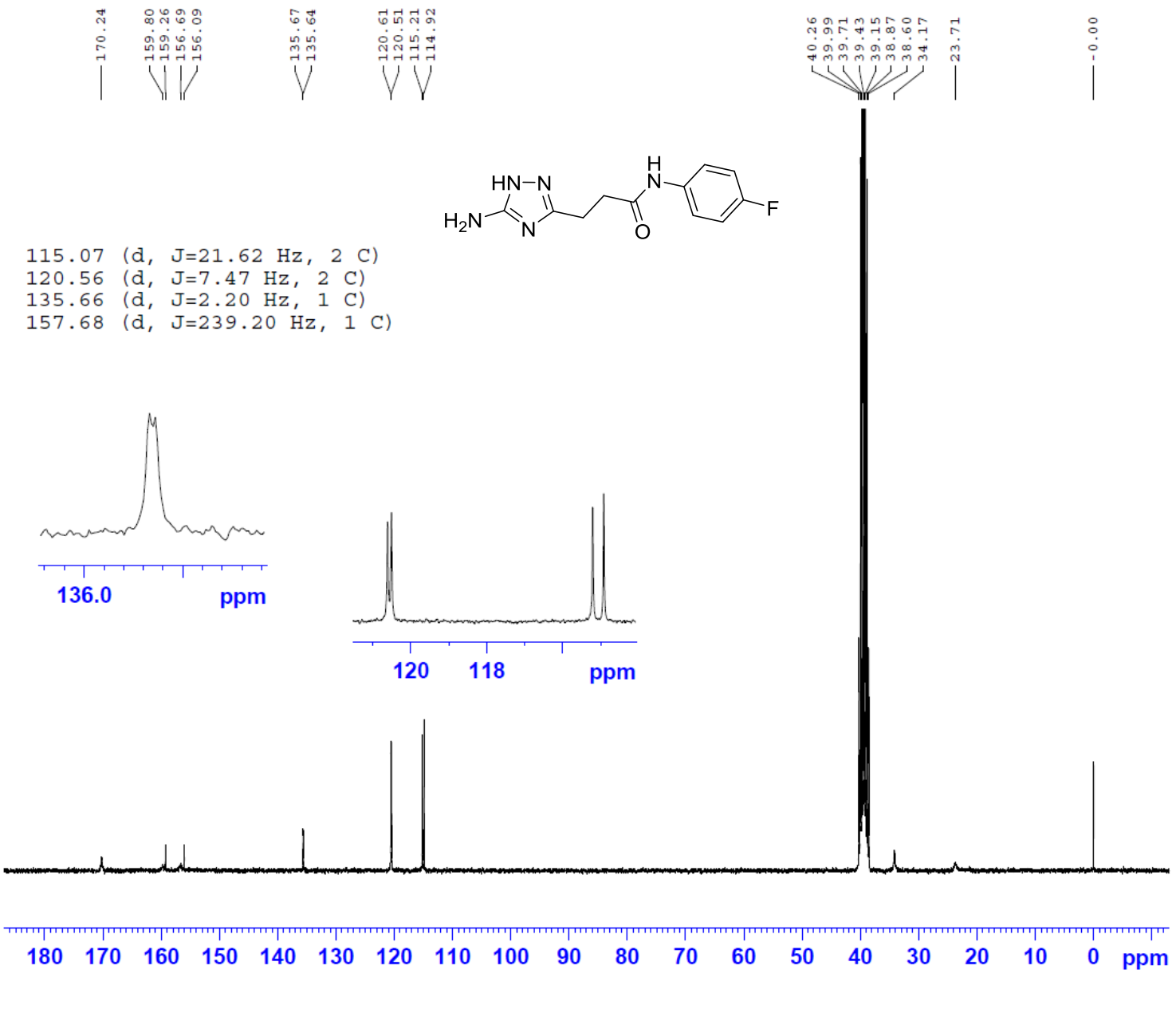

```
Current Data Parameters
NAME                  LY110
EXPNO                     4
PROCNO                    1

F2 - Acquisition Parameters
Date_              20171229
Time                  12.36
INSTRUM         FOURIER300
PROBHD     5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       16
DS                        2
SWH                6103.516 Hz
FIDRES            0.093132 Hz
AQ                5.3687091 sec
RG                  117.114
DW                   81.920 usec
DE                    6.50 usec
TE                   300.0 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           300.1618536 MHz
NUC1                     1H
P1                    13.50 usec
PLW1            9.30000019 W

F2 - Processing parameters
SI                    65536
SF             300.1599999 MHz
WDW                      EM
SSB         0
LB                    0.30 Hz
GB          0
PC                    1.00
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(4-fluorophenyl)propanamide (5k)




```
Current Data Parameters
NAME                  LY110
EXPNO                     5
PROCNO                    1

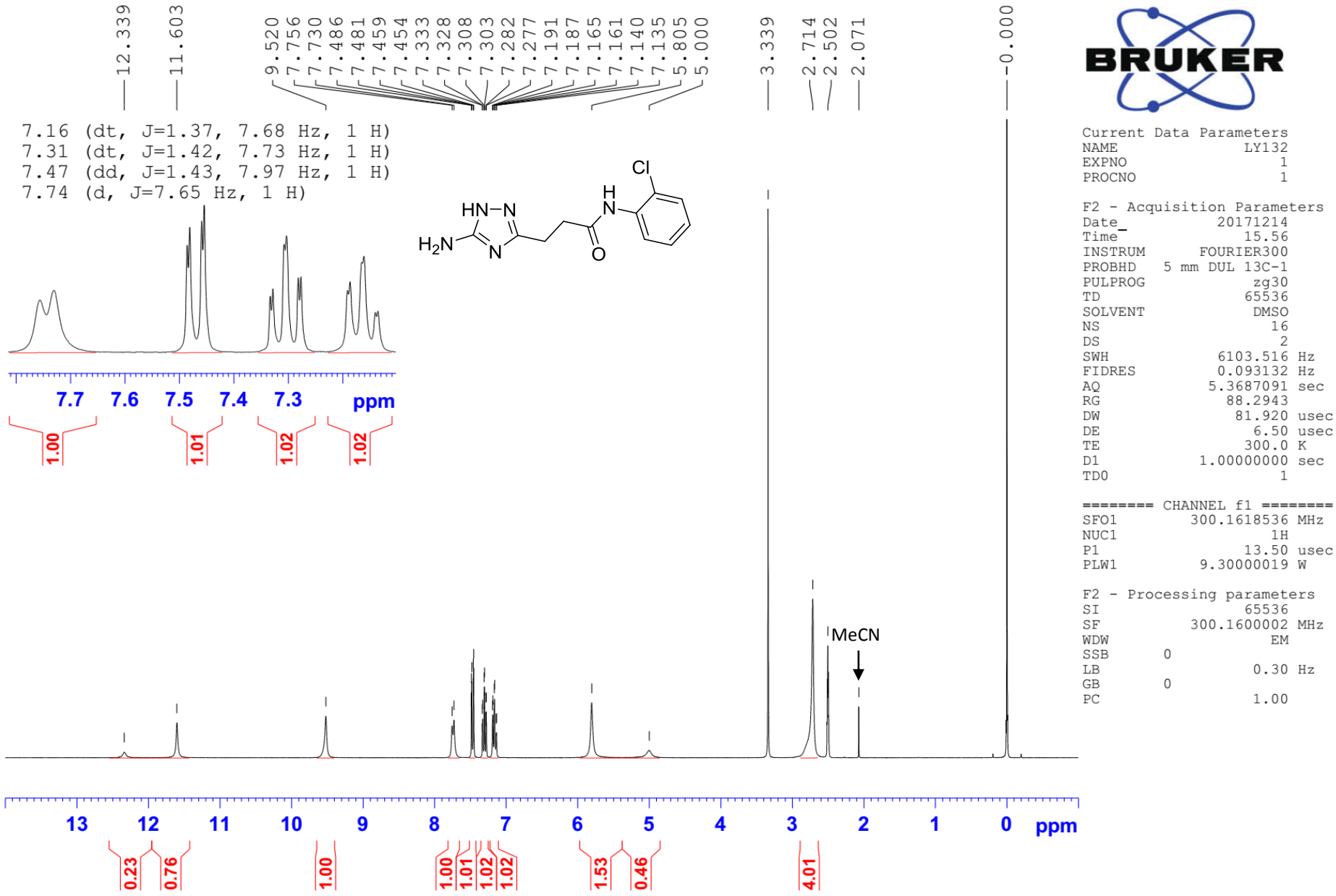
F2 - Acquisition Parameters
Date_              20171231
Time                   5.12
INSTRUM          FOURIER300
PROBHD     5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT               DMSO
NS                   15360
DS                       4
SWH             24414.063 Hz
FIDRES           0.372529 Hz
AQ               1.3421773 sec
RG                 501.187
DW                  20.480 usec
DE                   6.50 usec
TE                  300.0 K
D1              2.00000000 sec
D11             0.03000000 sec
D31             0.00001500 sec
D40             0.00439029 sec
L4                      37
L5                      53
P32                  98.00 usec
TD0                     15

======== CHANNEL f1 ========
SFO1            75.4828392 MHz
NUC1                   13C
P1                   15.00 usec
PLW1           22.00000000 W

======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                   1H
CPDPRG[2            waltz16
PCPD2                98.00 usec
PLW2            9.30000019 W
PLW12           0.29359001 W
PLW13           0.20359001 W

F2 - Processing parameters
SI                    32768
SF              75.4753344 MHz
WDW                      EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(2-chlorophenyl)propanamide (5l)



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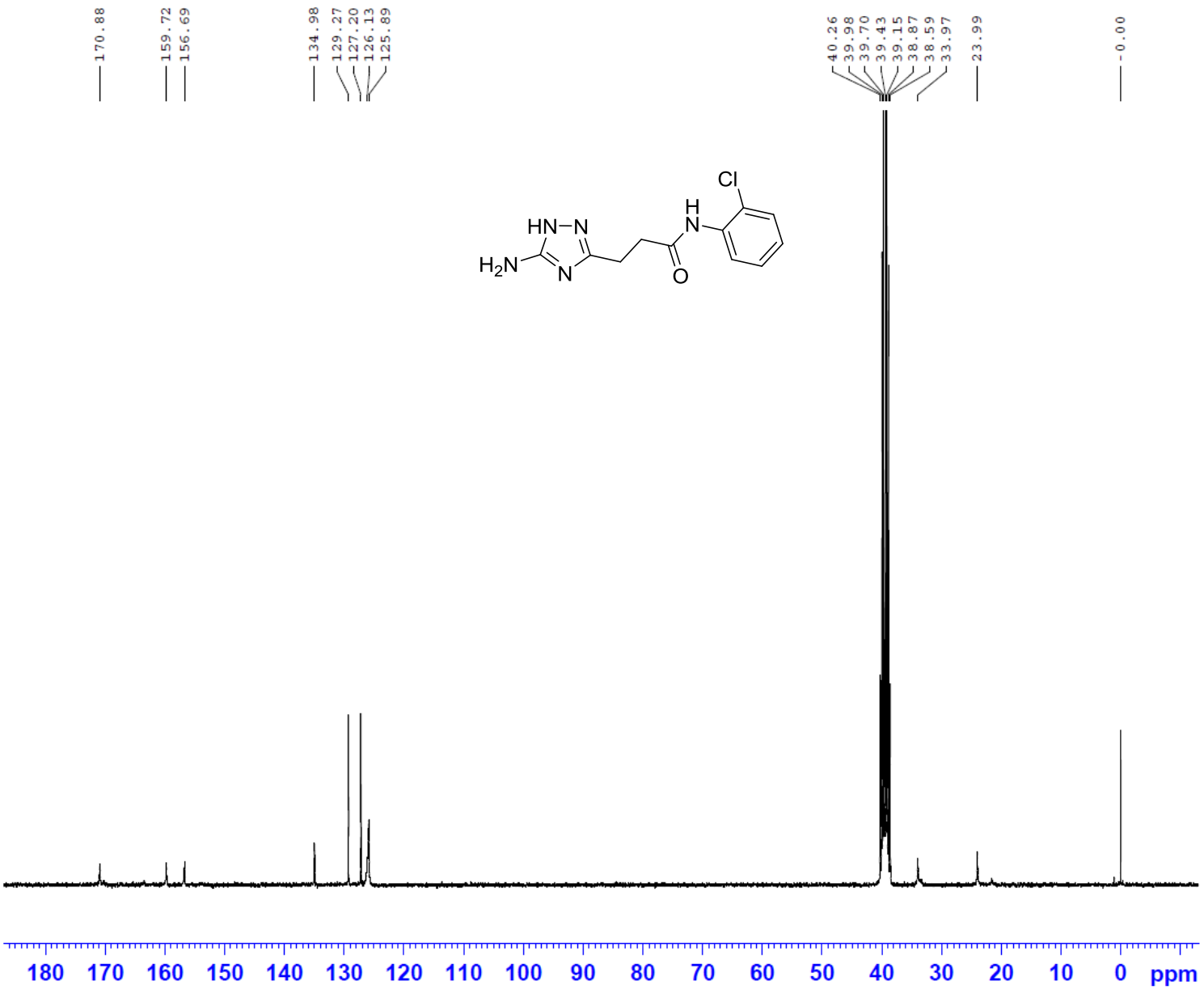
```
Current Data Parameters
NAME                  LY132
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20171214
Time                  15.56
INSTRUM         FOURIER300
PROBHD     5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT               DMSO
NS                       16
DS                        2
SWH                6103.516 Hz
FIDRES            0.093132 Hz
AQ                5.3687091 sec
RG                   88.2943
DW                  81.920 usec
DE                    6.50 usec
TE                   300.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1          300.1618536 MHz
NUC1                      1H
P1                    13.50 usec
PLW1           9.30000019 W

F2 - Processing parameters
SI                    65536
SF            300.1600002 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(2-chlorophenyl)propanamide (5l)



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```
Current Data Parameters
NAME                  LY132
EXPNO                     2
PROCNO                    1

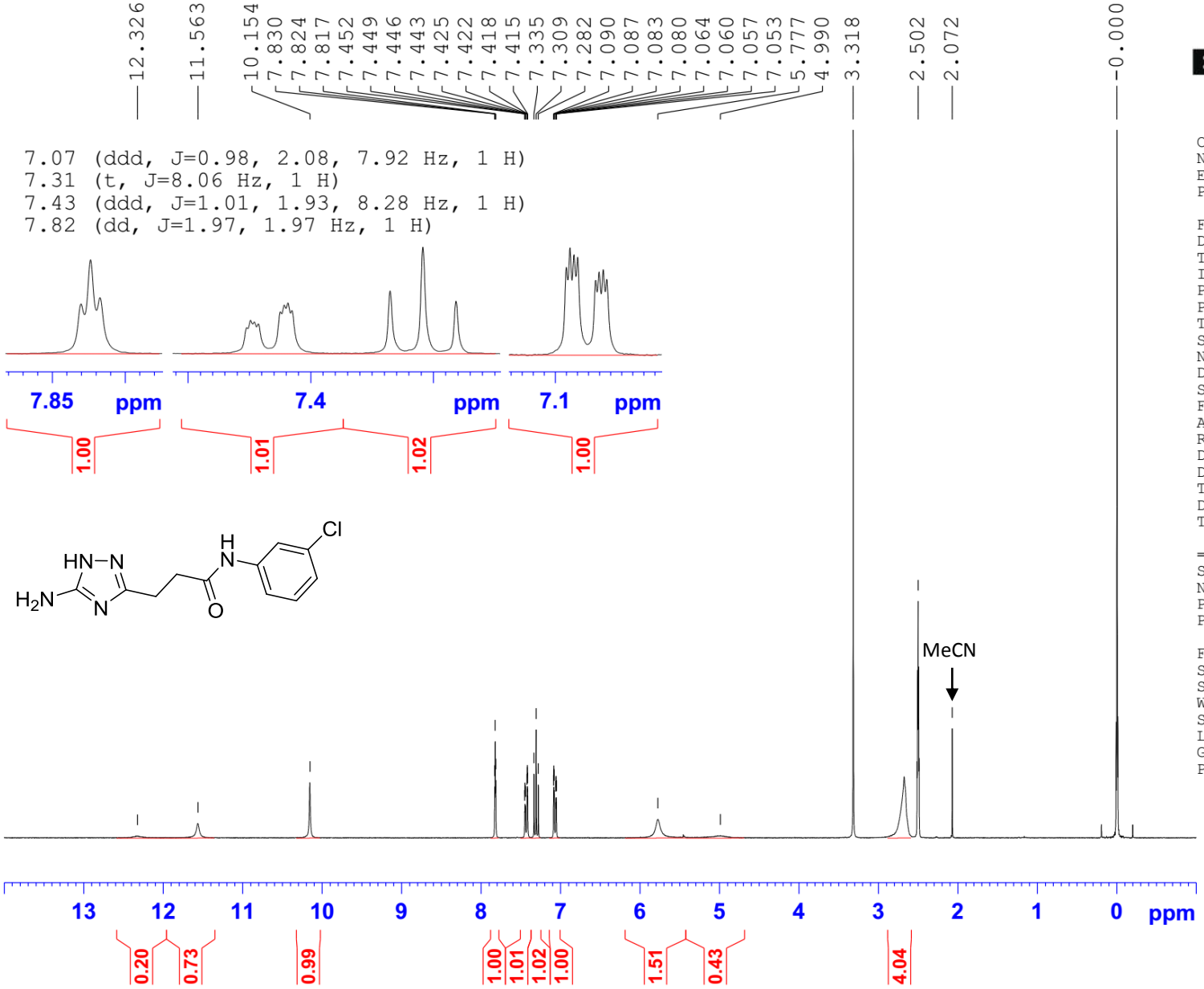
F2 - Acquisition Parameters
Date_              20171214
Time                  18.06
INSTRUM         FOURIER300
PROBHD     5 mm DUL 13C-1
PULPROG             zgpg30
TD                    65536
SOLVENT                DMSO
NS                    14336
DS                        4
SWH              24414.063 Hz
FIDRES            0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                 20.480 usec
DE                  6.50 usec
TE                  300.0 K
D1              2.00000000 sec
D11             0.03000000 sec
D31             0.00001500 sec
D40             0.00439029 sec
L4                       37
L5                       53
P32                98.00 usec
TD0                      14

======== CHANNEL f1 ========
SFO1            75.4828392 MHz
NUC1                    13C
P1                  15.00 usec
PLW1           22.00000000 W

======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                    1H
CPDPRG[2            waltz16
PCPD2               98.00 usec
PLW2            9.30000019 W
PLW12           0.29359001 W
PLW13           0.20359001 W

F2 - Processing parameters
SI                      32768
SF              75.4753350 MHz
WDW                        EM
SSB         0
LB                   1.00 Hz
GB          0
PC                   1.40
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(3-chlorophenyl)propanamide (5m)



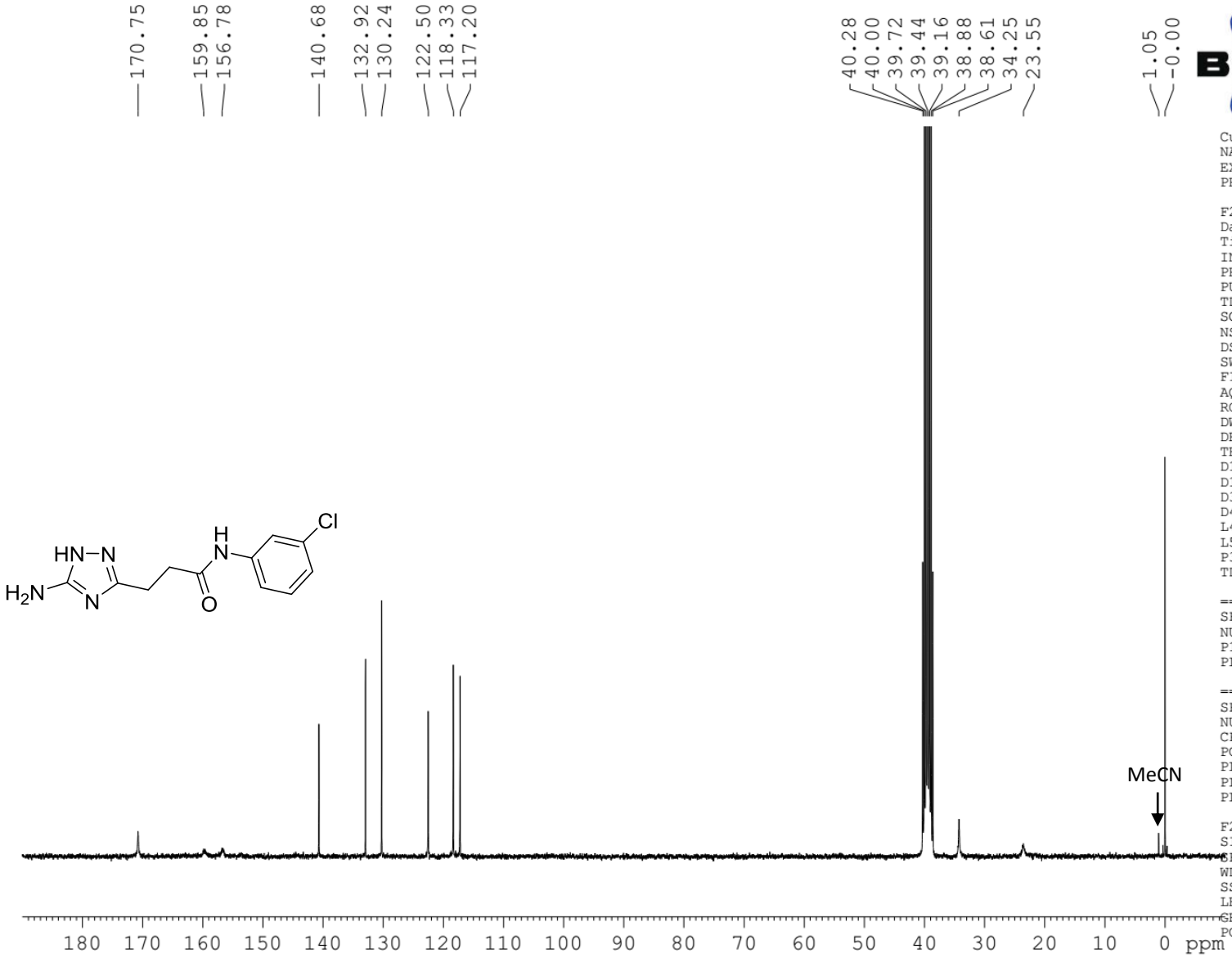

```
Current Data Parameters
NAME                  LY128
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20171227
Time                 10.48
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT               DMSO
NS                       16
DS                        2
SWH               6103.516 Hz
FIDRES           0.093132 Hz
AQ               5.3687091 sec
RG                  119.896
DW                   81.920 usec
DE                    6.50 usec
TE                   300.0 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1          300.1618536 MHz
NUC1                     1H
P1                    13.50 usec
PLW1           9.30000019 W

F2 - Processing parameters
SI                    65536
SF            300.1600002 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(3-chlorophenyl)propanamide (5m)




```
Current Data Parameters
NAME                  LY128
EXPNO                     2
PROCNO                    1

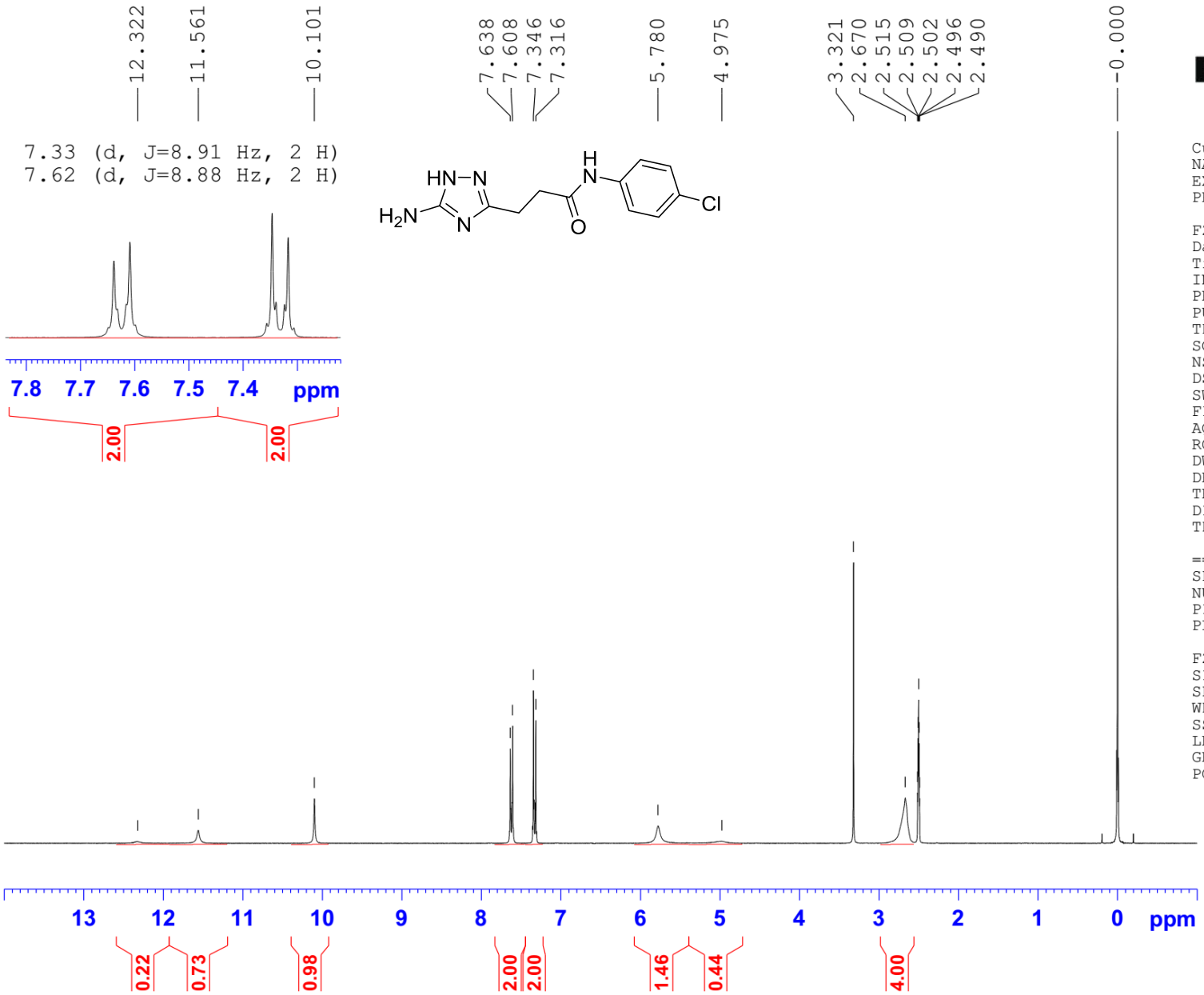
F2 - Acquisition Parameters
Date_              20171212
Time                  21.53
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                    65536
SOLVENT                DMSO
NS                    14336
DS                        4
SWH              24414.063 Hz
FIDRES            0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                   20.480 usec
DE                    6.50 usec
TE                   300.0 K
D1              2.00000000 sec
D11             0.03000000 sec
D31             0.00001500 sec
D40             0.00439029 sec
L4                       37
L5                       53
P32                   98.00 usec
TD0                      14

======== CHANNEL f1 ========
SFO1            75.4828392 MHz
NUC1                    13C
P1                    15.00 usec
PLW1           22.00000000 W

======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2                 98.00 usec
PLW2            9.30000019 W
PLW12           0.29359001 W
PLW13           0.20359001 W

F2 - Processing parameters
SI                     32768
SF              75.4753343 MHz
WDW                       EM
SSB         0
LB                     1.00 Hz
GB          0
PC                     1.40
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(4-chlorophenyl)propanamide (5n)



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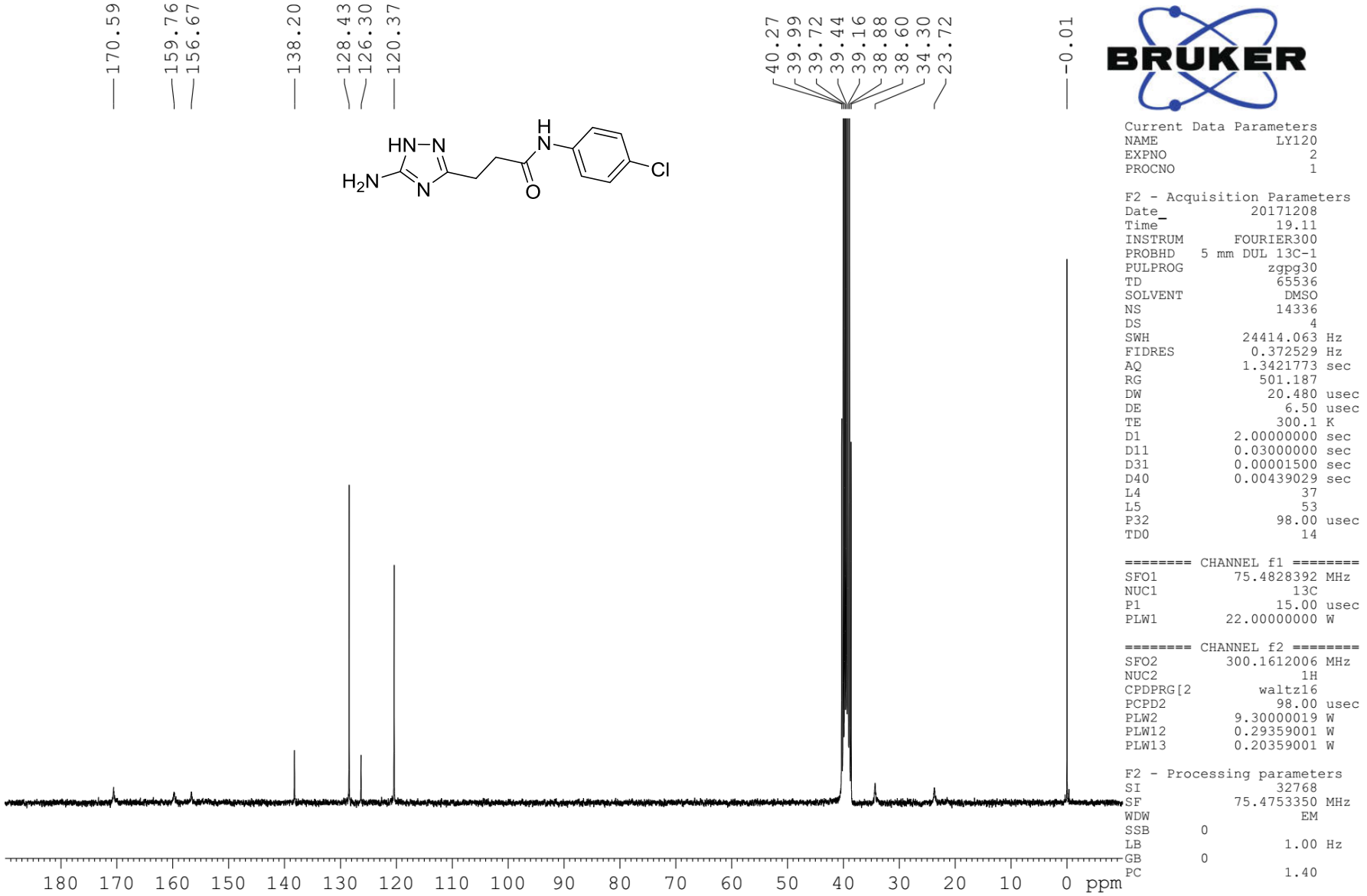
```
Current Data Parameters
NAME                  LY120
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20171208
Time                  14.04
INSTRUM         FOURIER300
PROBHD     5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT               DMSO
NS                       16
DS                        2
SWH                6103.516 Hz
FIDRES            0.093132 Hz
AQ                5.3687091 sec
RG                  94.6841
DW                  81.920 usec
DE                    6.50 usec
TE                   300.0 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           300.1618536 MHz
NUC1                     1H
P1                    13.50 usec
PLW1           9.30000019 W

F2 - Processing parameters
SI                   65536
SF             300.1599999 MHz
WDW                     EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(4-chlorophenyl)propanamide (5n)



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```
Current Data Parameters
NAME                  LY120
EXPNO                     2
PROCNO                    1

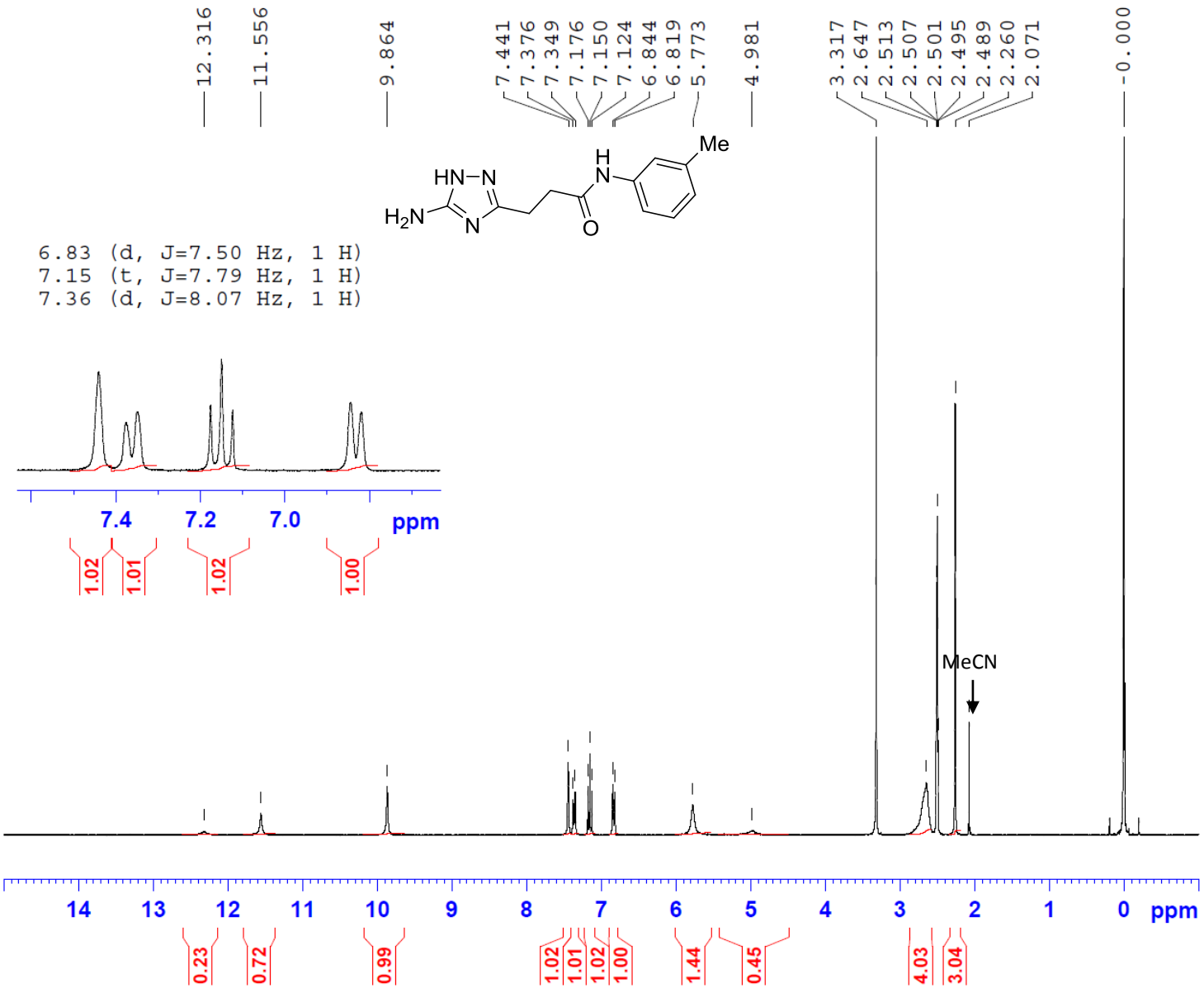
F2 - Acquisition Parameters
Date_              20171208
Time                  19.11
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                   14336
DS                       4
SWH              24414.063 Hz
FIDRES            0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                   20.480 usec
DE                    6.50 usec
TE                   300.1 K
D1               2.00000000 sec
D11              0.03000000 sec
D31              0.00001500 sec
D40              0.00439029 sec
L4                       37
L5                       53
P32                   98.00 usec
TD0                      14

======== CHANNEL f1 ========
SFO1            75.4828392 MHz
NUC1                    13C
P1                    15.00 usec
PLW1           22.00000000 W

======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2                 98.00 usec
PLW2            9.30000019 W
PLW12           0.29359001 W
PLW13           0.20359001 W

F2 - Processing parameters
SI                    32768
SF              75.4753350 MHz
WDW                      EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(3-methylphenyl)propanamide (5o)



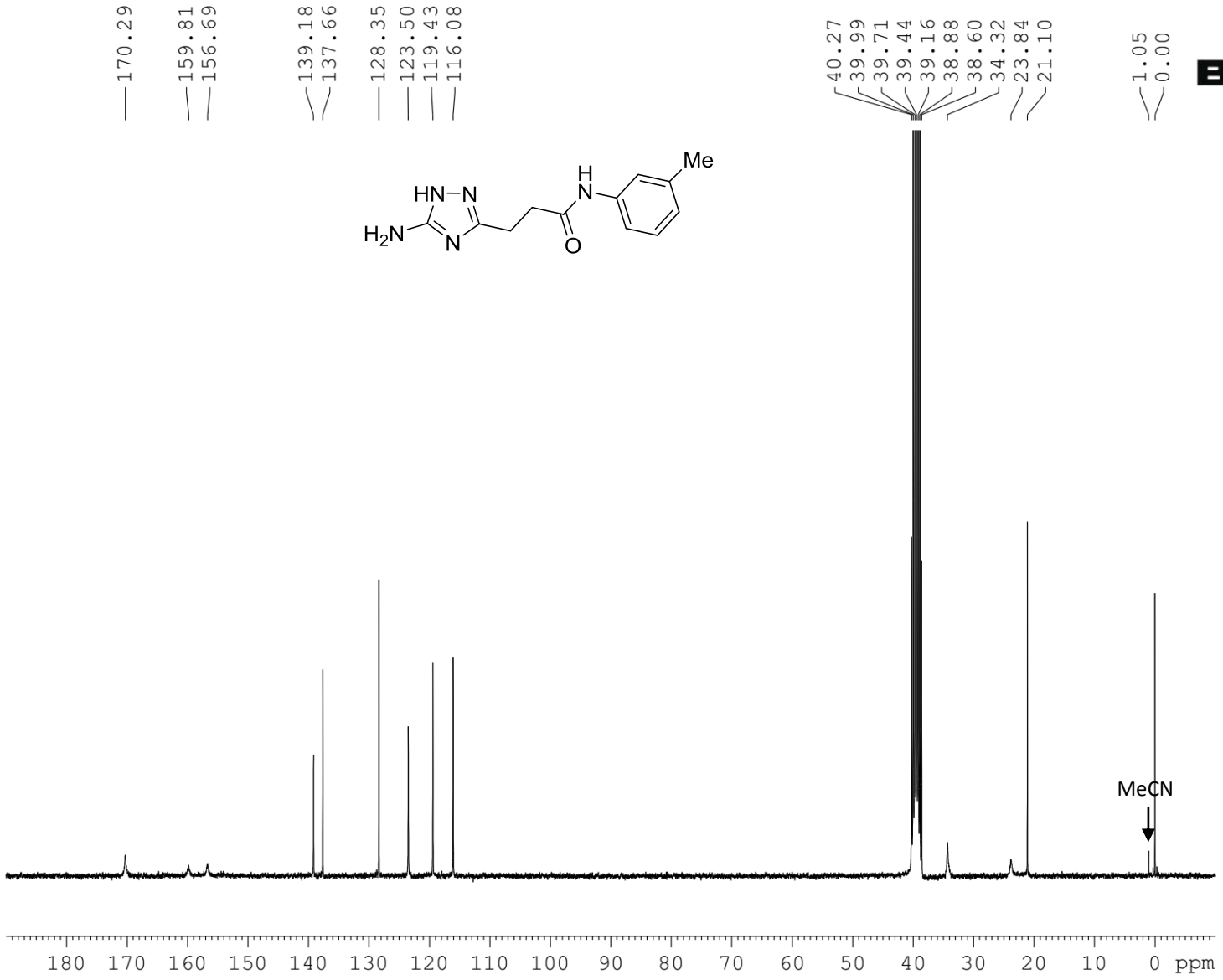

```
Current Data Parameters
NAME                  LY123
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20171228
Time                 16.24
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT               DMSO
NS                       16
DS                        2
SWH               6103.516 Hz
FIDRES            0.093132 Hz
AQ                5.3687091 sec
RG                  116.552
DW                   81.920 usec
DE                    6.50 usec
TE                   300.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1          300.1618536 MHz
NUC1                    1H
P1                   13.50 usec
PLW1           9.30000019 W

F2 - Processing parameters
SI                   65536
SF            300.1600003 MHz
WDW                     EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(3-methylphenyl)propanamide (5o)



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```
Current Data Parameters
NAME                  LY123
EXPNO                     2
PROCNO                    1

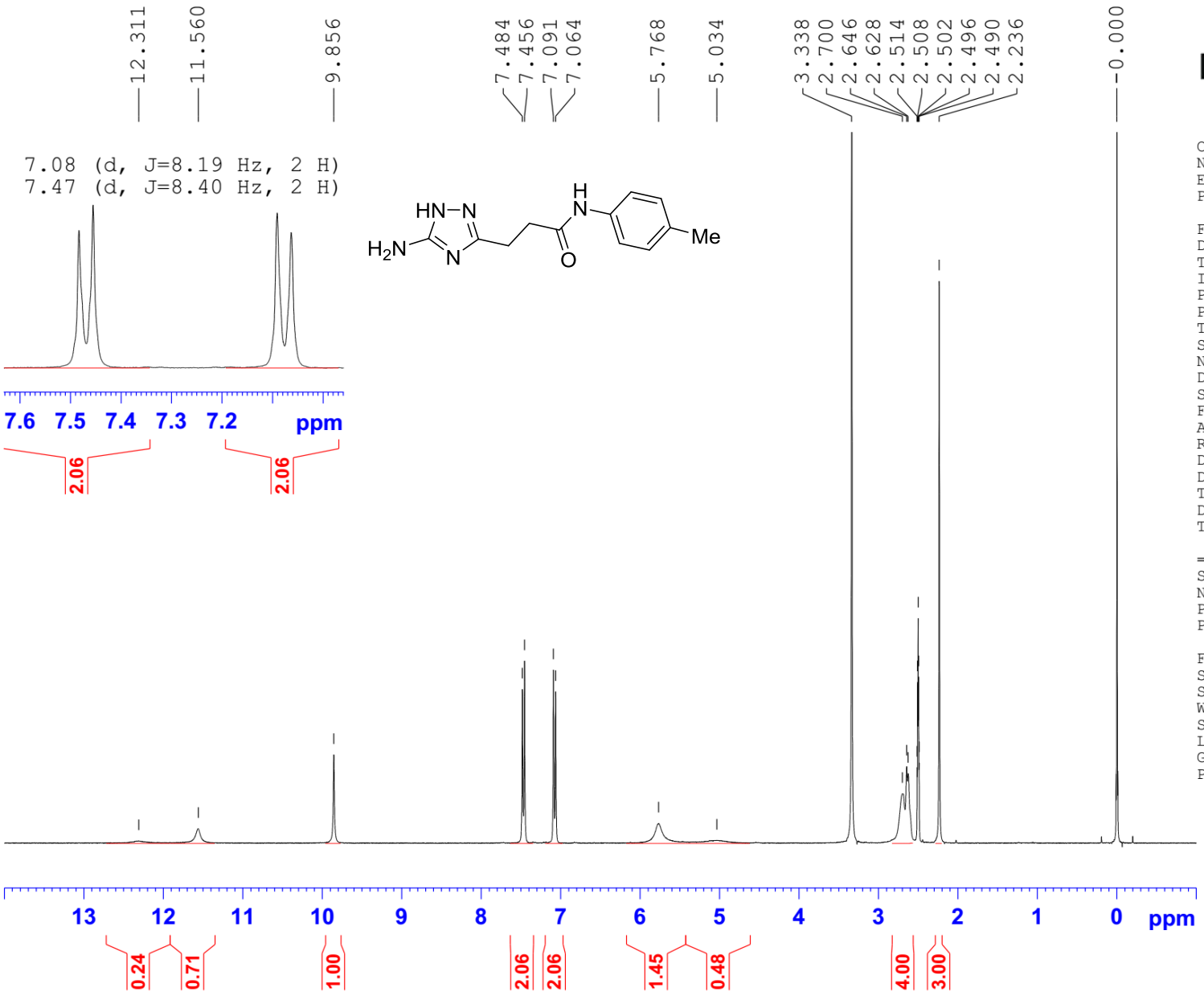
F2 - Acquisition Parameters
Date_              20171211
Time                  19.43
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT               DMSO
NS                   14336
DS                       4
SWH             24414.063 Hz
FIDRES           0.372529 Hz
AQ               1.3421773 sec
RG                 501.187
DW                  20.480 usec
DE                   6.50 usec
TE                  300.1 K
D1              2.00000000 sec
D11             0.03000000 sec
D31             0.00001500 sec
D40             0.00439029 sec
L4                      37
L5                      53
P32                  98.00 usec
TD0                     14

======== CHANNEL f1 ========
SFO1            75.4828392 MHz
NUC1                   13C
P1                   15.00 usec
PLW1          22.00000000 W

======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2                98.00 usec
PLW2            9.30000019 W
PLW12           0.29359001 W
PLW13           0.20359001 W

F2 - Processing parameters
SI                    32768
SF              75.4753344 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(4-methylphenyl)propanamide (5p)



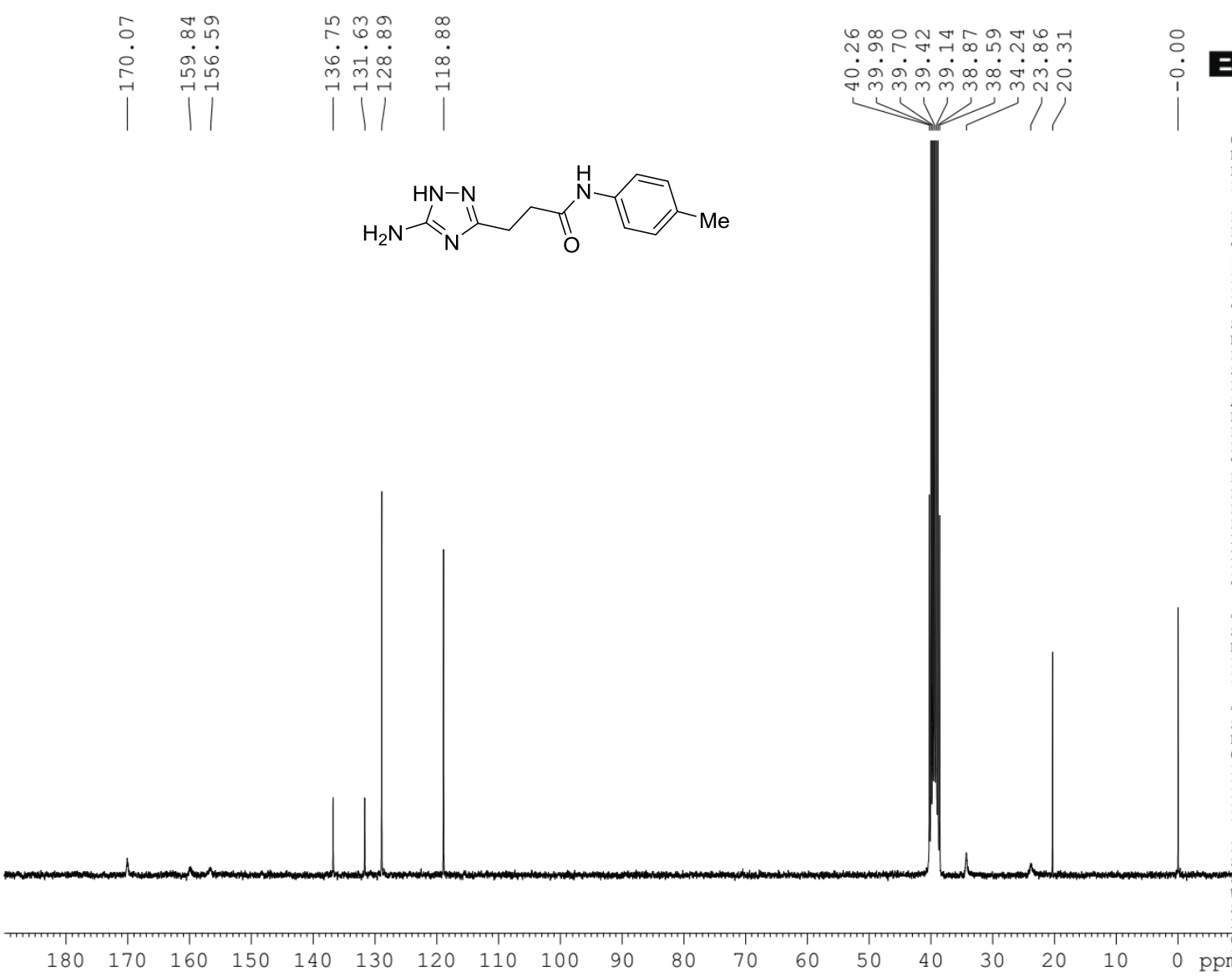

```
Current Data Parameters
NAME                  LY106
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20171203
Time                  19.30
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       16
DS                        2
SWH                6103.516 Hz
FIDRES            0.093132 Hz
AQ                5.3687091 sec
RG                   83.6023
DW                  81.920 usec
DE                   6.50 usec
TE                  300.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1          300.1618536 MHz
NUC1                      1H
P1                    13.50 usec
PLW1           9.30000019 W

F2 - Processing parameters
SI                    65536
SF            300.1600002 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(4-methylphenyl)propanamide (5p)




```
Current Data Parameters
NAME                  LY106
EXPNO                     3
PROCNO                    1

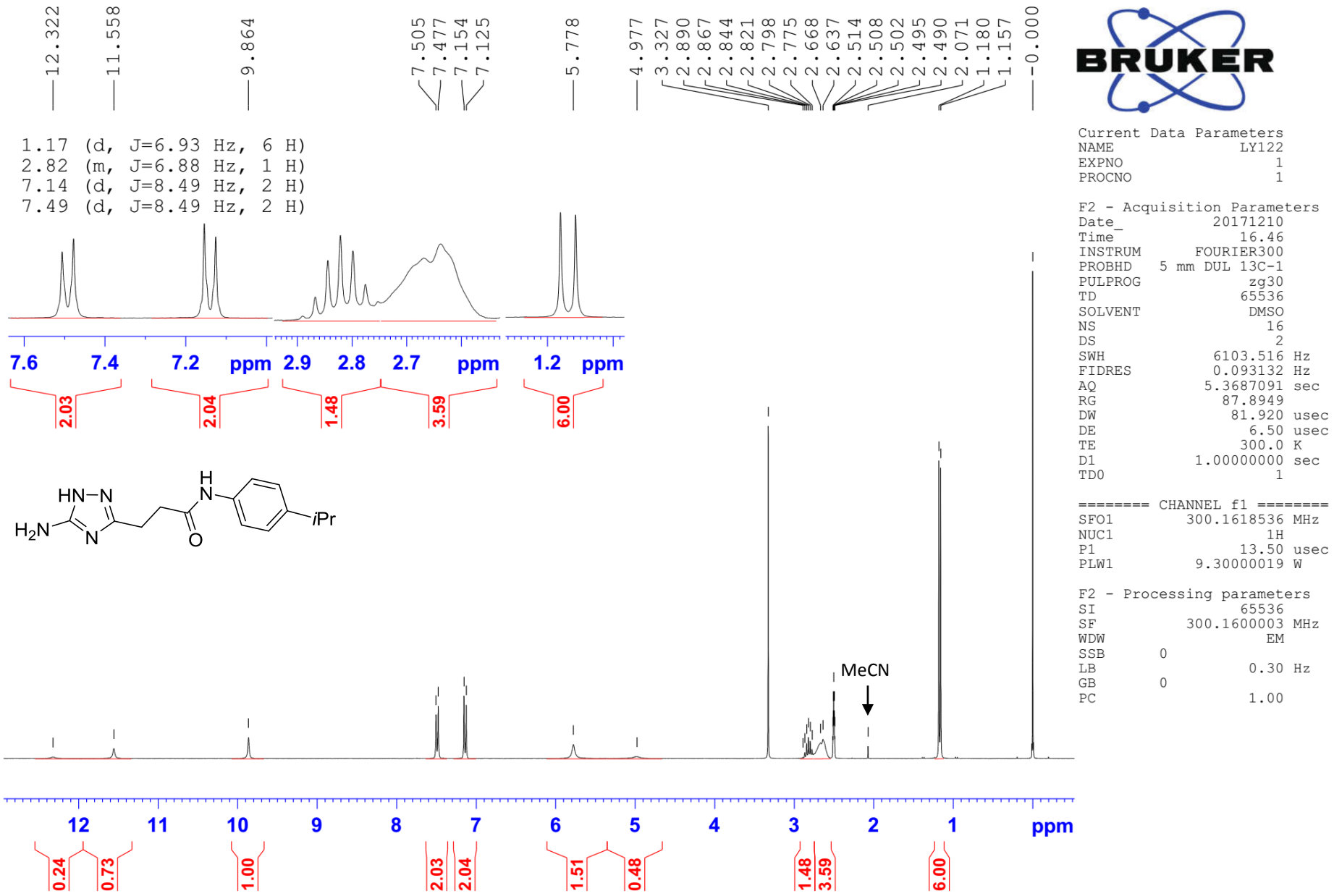
F2 - Acquisition Parameters
Date_              20171203
Time                  19.49
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                    65536
SOLVENT                DMSO
NS                    14336
DS                        4
SWH              24414.063 Hz
FIDRES            0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                   20.480 usec
DE                    6.50 usec
TE                   300.0 K
D1               2.00000000 sec
D11              0.03000000 sec
D31              0.00001500 sec
D40              0.00439029 sec
L4                       37
L5                       53
P32                   98.00 usec
TD0                      14

======== CHANNEL f1 ========
SFO1            75.4828392 MHz
NUC1                    13C
P1                    15.00 usec
PLW1           22.00000000 W

======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2                 98.00 usec
PLW2            9.30000019 W
PLW12           0.29359001 W
PLW13           0.20359001 W

F2 - Processing parameters
SI                     32768
SF              75.4753350 MHz
WDW                       EM
SSB         0
LB                     1.00 Hz
GB          0
PC                     1.40
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(4-isopropylphenyl)propanamide (5q)



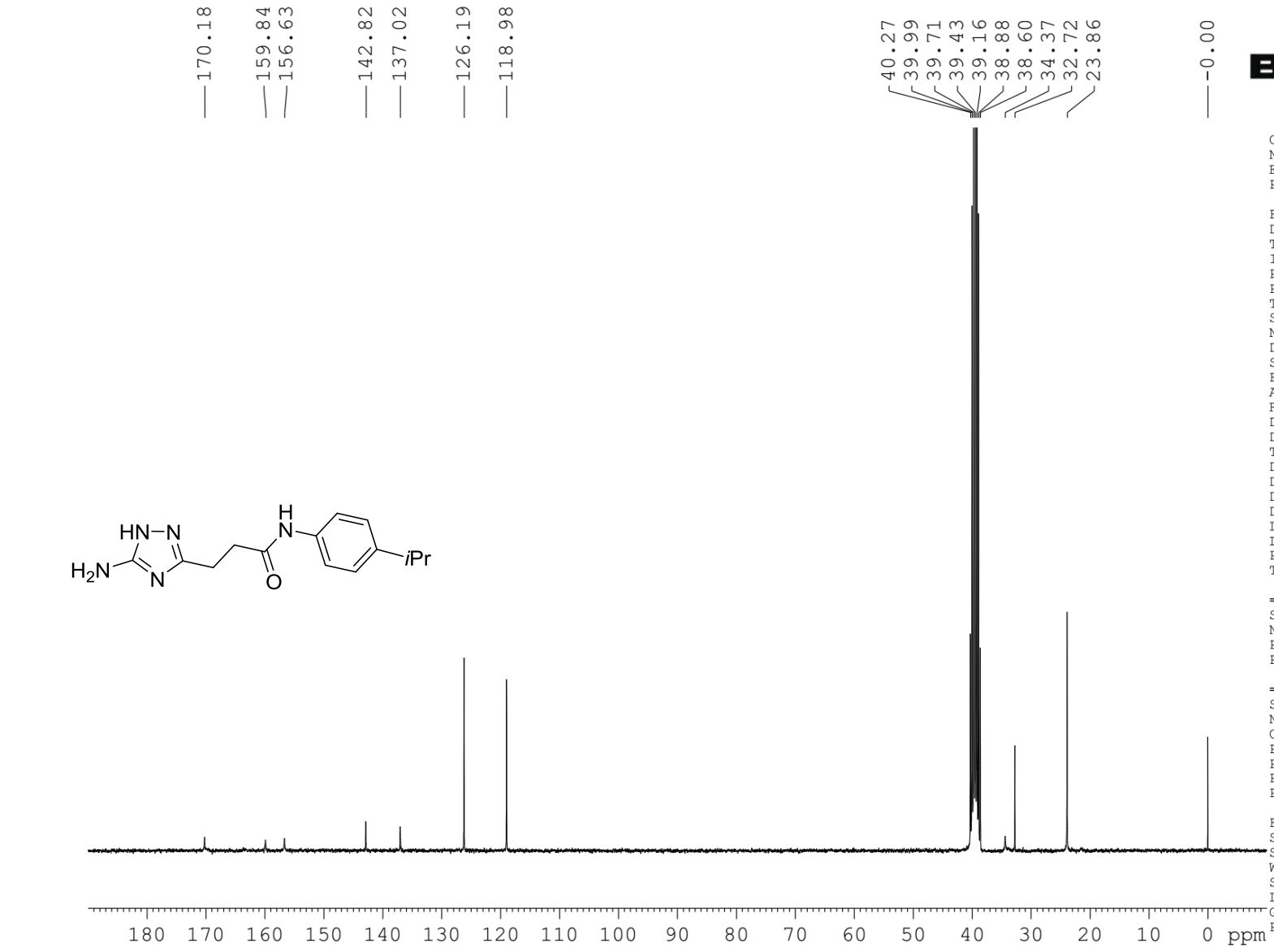

```
Current Data Parameters
NAME                  LY122
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20171210
Time                  16.46
INSTRUM         FOURIER300
PROBHD     5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT               DMSO
NS                       16
DS                        2
SWH                6103.516 Hz
FIDRES             0.093132 Hz
AQ                 5.3687091 sec
RG                   87.8949
DW                   81.920 usec
DE                    6.50 usec
TE                   300.0 K
D1                 1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1            300.1618536 MHz
NUC1                      1H
P1                    13.50 usec
PLW1            9.30000019 W

F2 - Processing parameters
SI                   65536
SF              300.1600003 MHz
WDW                     EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(4-isopropylphenyl)propanamide (5q)



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```
Current Data Parameters
NAME                 LY122
EXPNO                    2
PROCNO                   1

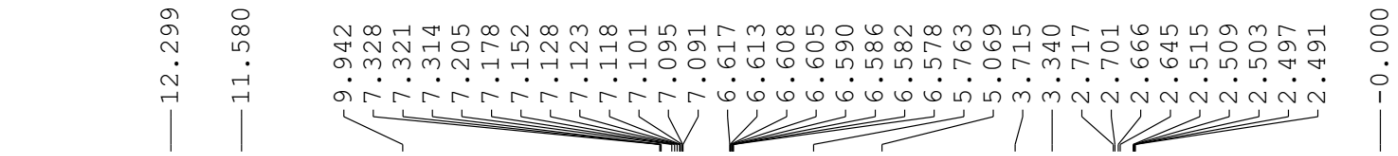
F2 - Acquisition Parameters
Date_             20171210
Time                 17.10
INSTRUM       FOURIER300
PROBHD   5 mm DUL 13C-1
PULPROG            zgpg30
TD                  65536
SOLVENT               DMSO
NS                  14336
DS                      4
SWH             24414.063 Hz
FIDRES           0.372529 Hz
AQ               1.3421773 sec
RG                 501.187
DW                  20.480 usec
DE                   6.50 usec
TE                  300.1 K
D1              2.00000000 sec
D11             0.03000000 sec
D31             0.00001500 sec
D40             0.00439029 sec
L4                      37
L5                      53
P32                 98.00 usec
TD0                     14

======== CHANNEL f1 ========
SFO1           75.4828392 MHz
NUC1                   13C
P1                  15.00 usec
PLW1          22.00000000 W

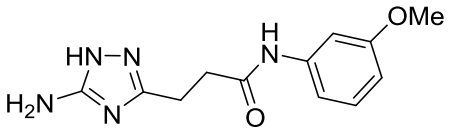
======== CHANNEL f2 ========
SFO2          300.1612006 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2               98.00 usec
PLW2           9.30000019 W
PLW12          0.29359001 W
PLW13          0.20359001 W

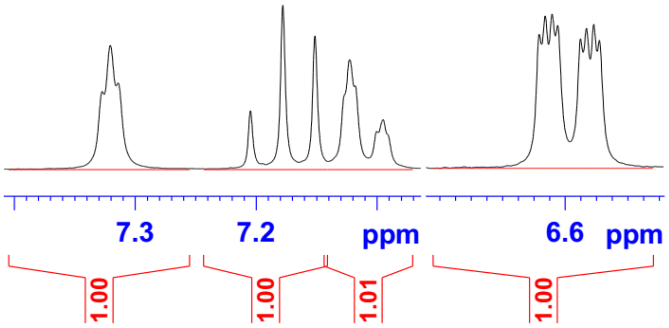
F2 - Processing parameters
SI                    32768
SF             75.4753350 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

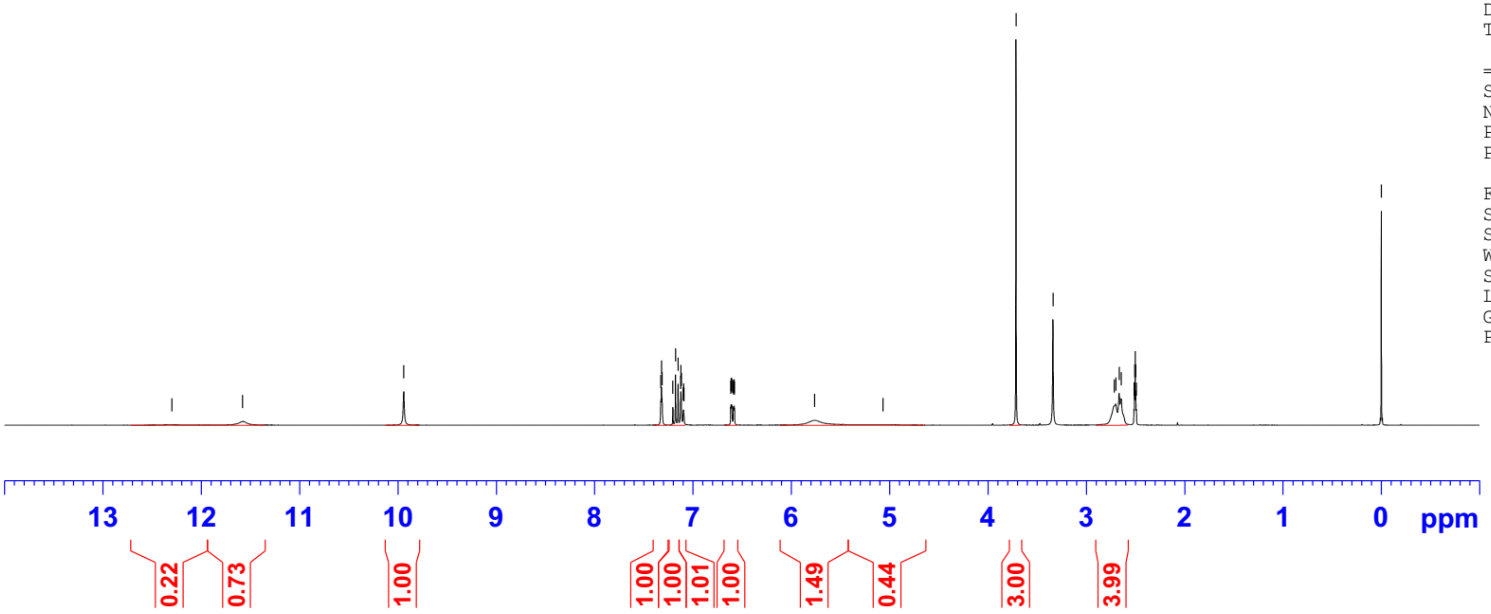
3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(3-methoxyphenyl)propanamide (5r)



6.60 (ddd, J=1.11, 2.46, 7.95 Hz, 1 H)
7.11 (ddd, J=1.46, 1.46, 8.29 Hz, 1 H)
7.18 (t, J=8.01 Hz, 1 H)
7.32 (dd, J=1.98, 1.98 Hz, 1 H)







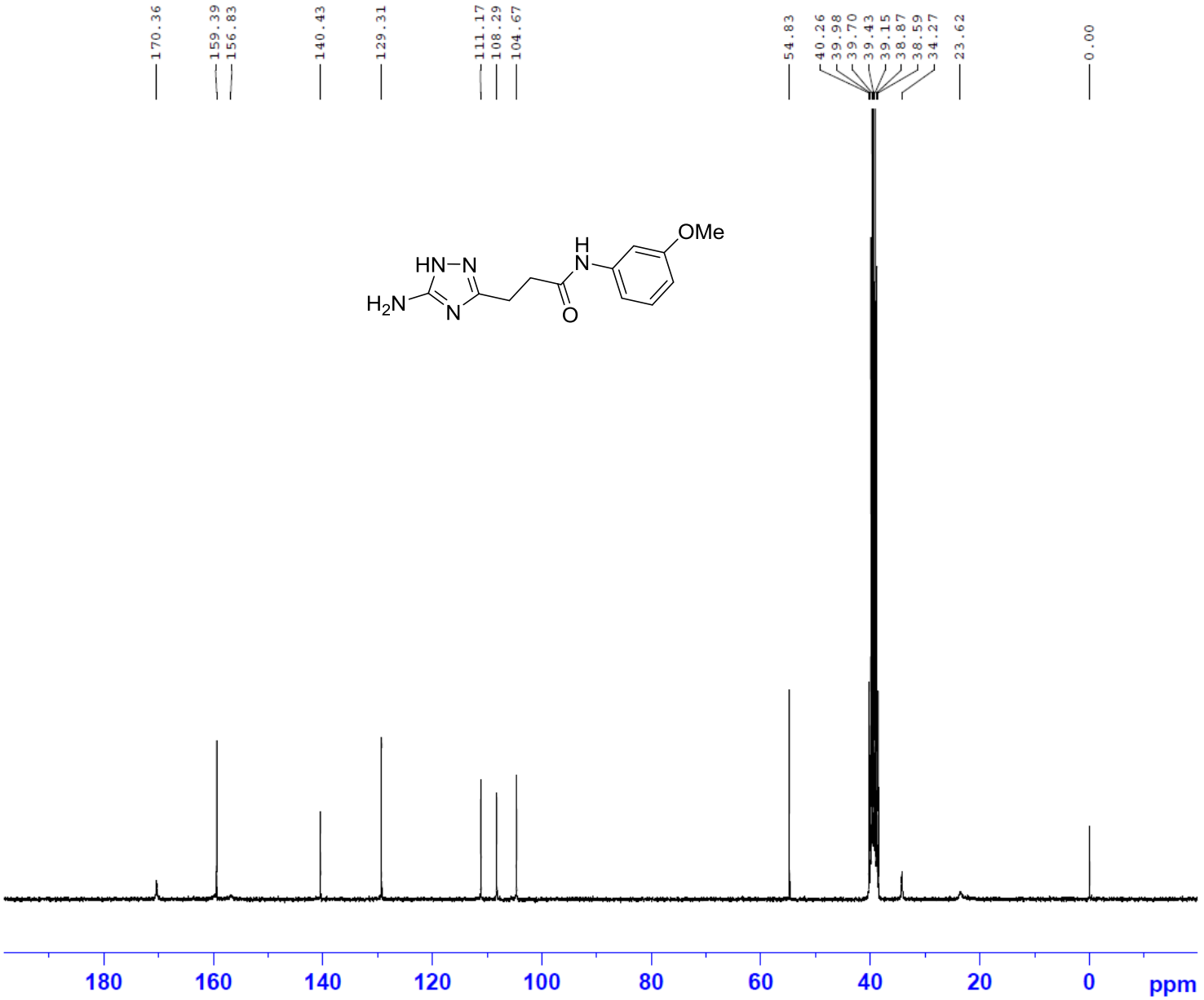

```
Current Data Parameters
NAME                  LY140
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20171219
Time                  13.29
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT               DMSO
NS                      16
DS                       2
SWH               6103.702 Hz
FIDRES           0.093135 Hz
AQ               5.3685451 sec
RG                  141.254
DW                   81.918 usec
DE                     6.50 usec
TE                    300.0 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           300.1618536 MHz
NUC1                   1H
P1                    13.50 usec
PLW1           9.30000019 W

F2 - Processing parameters
SI                    65536
SF             300.1599999 MHz
WDW                     EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(3-methoxyphenyl)propanamide (5r)



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```
Current Data Parameters
NAME                  LY140
EXPNO                     2
PROCNO                    1

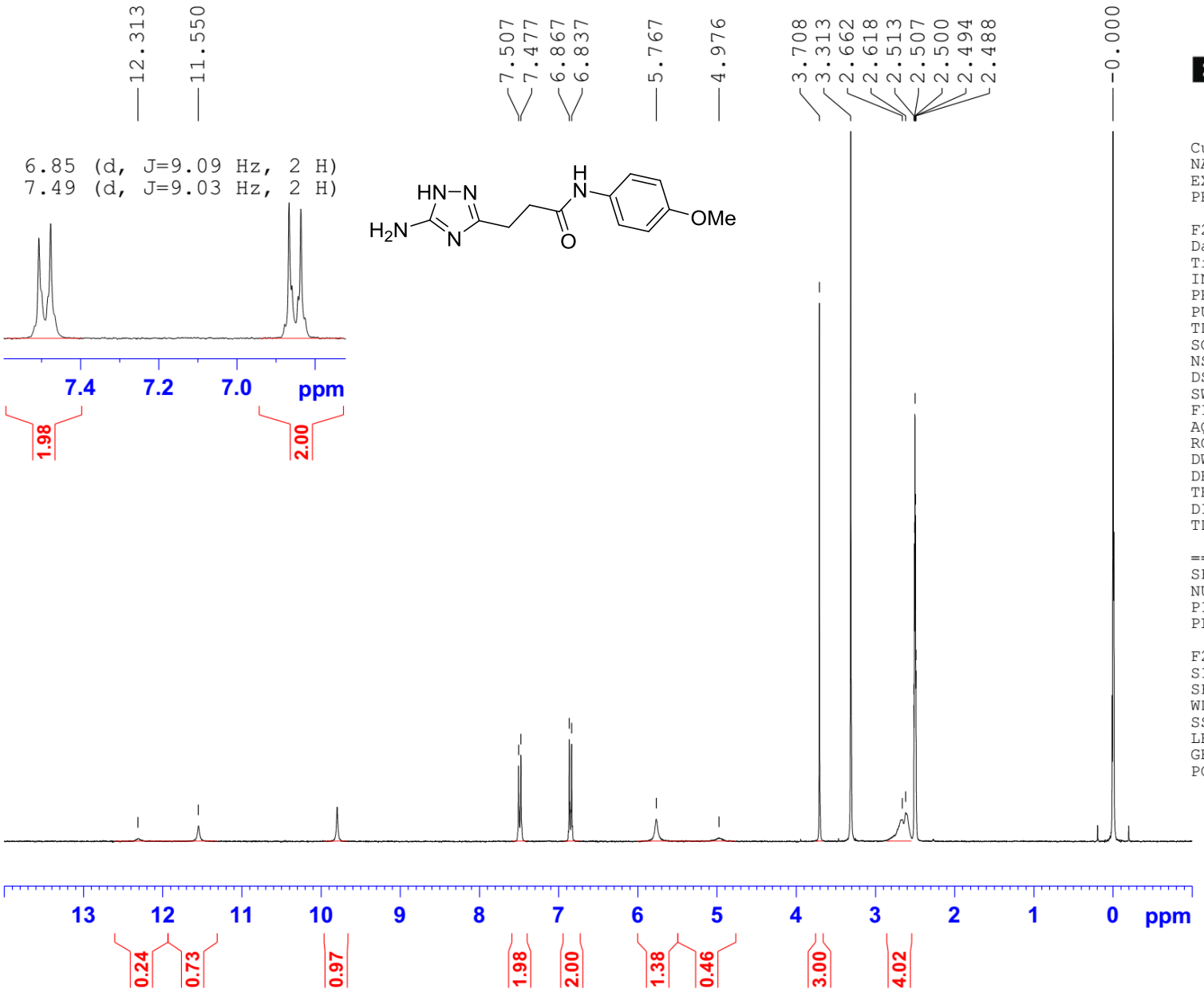
F2 - Acquisition Parameters
Date_              20171227
Time                  19.30
INSTRUM          FOURIER300
PROBHD     5 mm DUL 13C-1
PULPROG              zgpg30
TD                    65536
SOLVENT                DMSO
NS                    14336
DS                        4
SWH              24414.063 Hz
FIDRES            0.372529 Hz
AQ                1.3421773 sec
RG                  501.187
DW                 20.480 usec
DE                  6.50 usec
TE                  300.1 K
D1              2.00000000 sec
D11             0.03000000 sec
D31             0.00001500 sec
D40             0.00439029 sec
L4                       37
L5                       53
P32                98.00 usec
TD0                      14

======== CHANNEL f1 ========
SFO1            75.4828392 MHz
NUC1                    13C
P1                  15.00 usec
PLW1           22.00000000 W

======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2               98.00 usec
PLW2            9.30000019 W
PLW12           0.29359001 W
PLW13           0.20359001 W

F2 - Processing parameters
SI                    32768
SF              75.4753345 MHz
WDW                     EM
SSB         0
LB                   1.00 Hz
GB          0
PC                   1.40
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(4-methoxyphenyl)propanamide (5s)



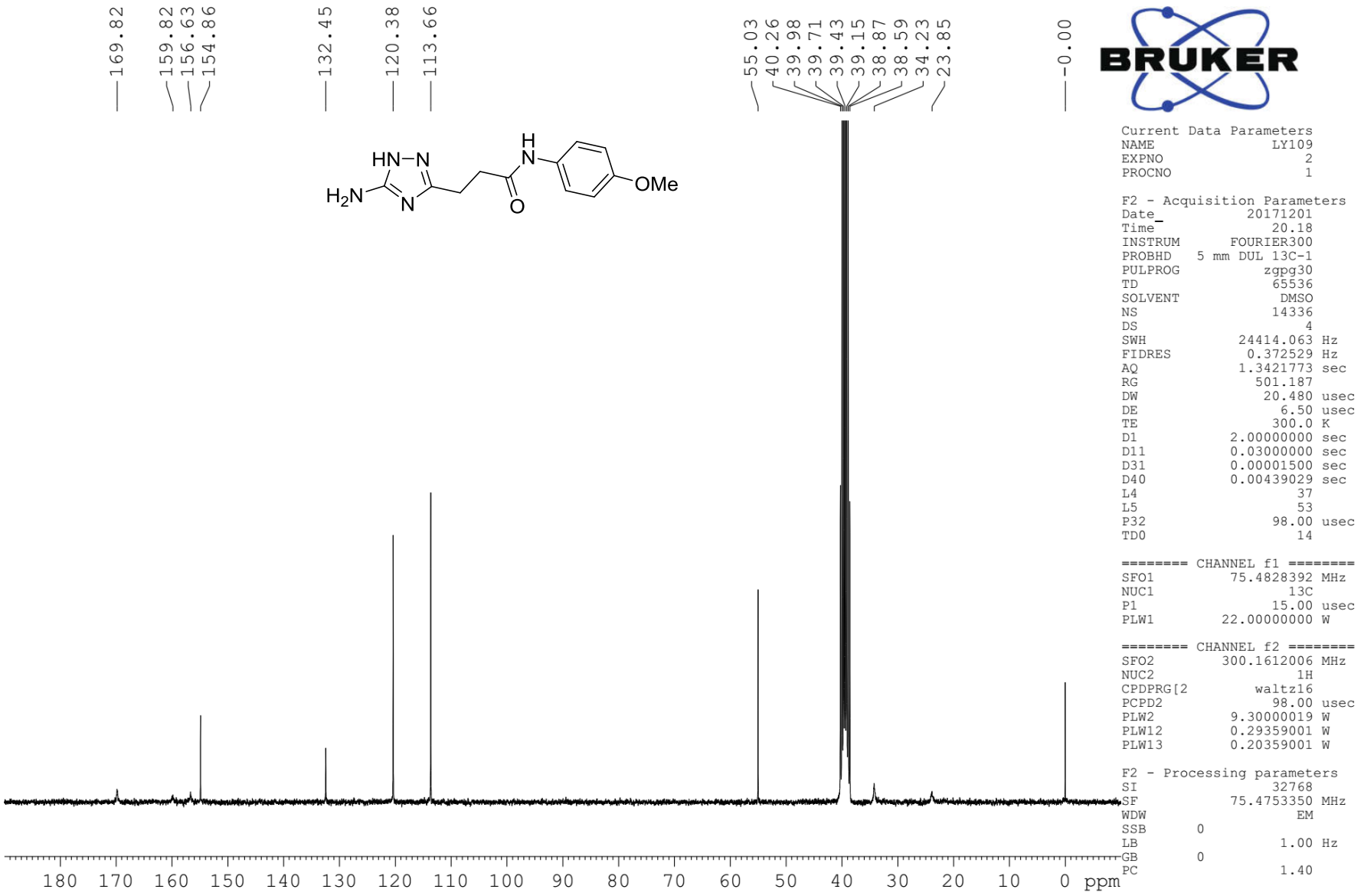

```
Current Data Parameters
NAME                  LY109
EXPNO                     3
PROCNO                    1

F2 - Acquisition Parameters
Date_              20171226
Time                  16.14
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       16
DS                        2
SWH                6103.516 Hz
FIDRES            0.093132 Hz
AQ                5.3687091 sec
RG                  158.089
DW                   81.920 usec
DE                    6.50 usec
TE                   300.0 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           300.1618536 MHz
NUC1                     1H
P1                    13.50 usec
PLW1           9.30000019 W

F2 - Processing parameters
SI                    65536
SF             300.1600008 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(4-methoxyphenyl)propanamide (5s)



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Current Data Parameters
NAME LY109
EXPNO 2
PROCNO 1

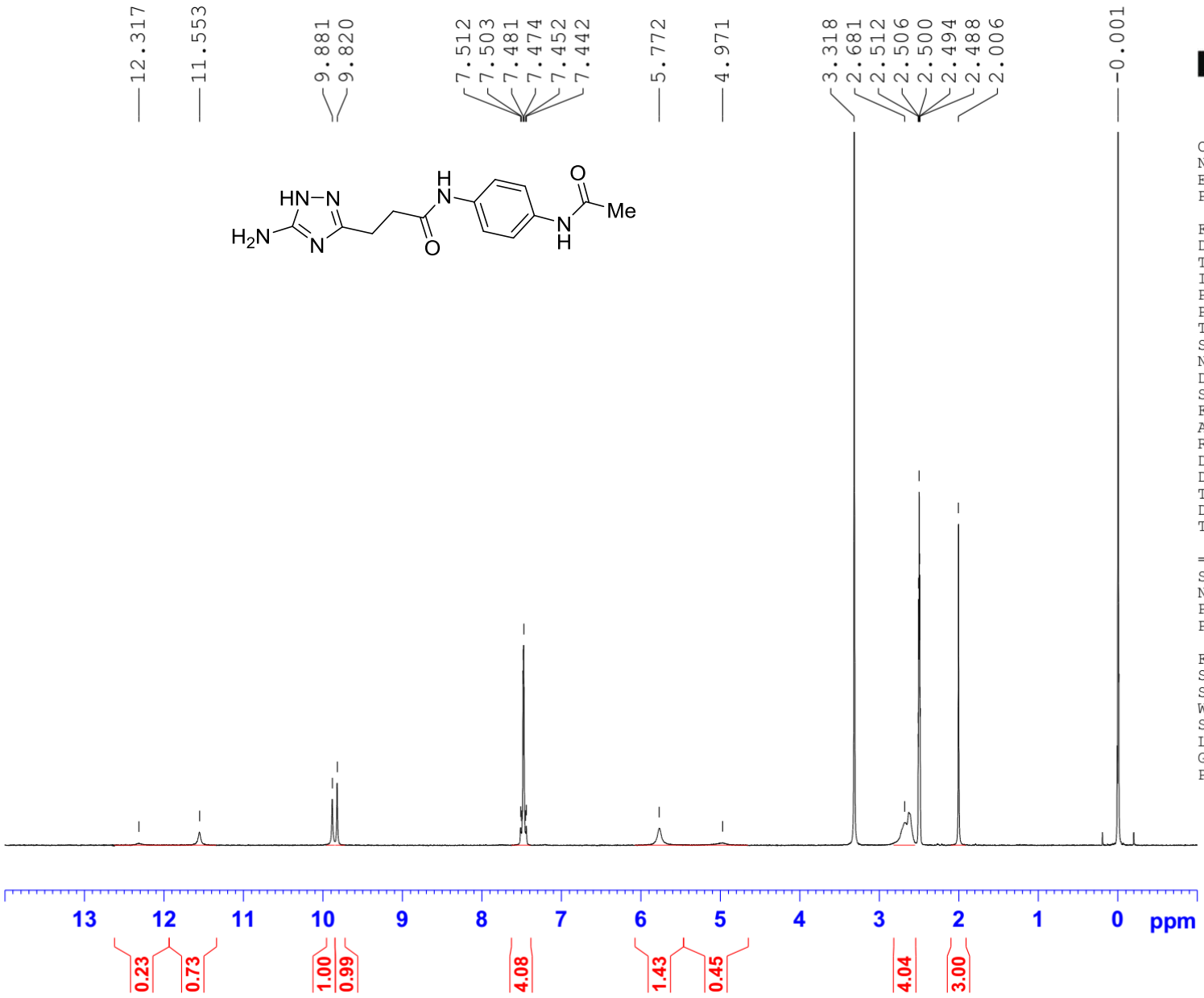
F2 - Acquisition Parameters
Date_ 20171201
Time 20.18
INSTRUM FOURIER300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 14336
DS 4
SWH 24414.063 Hz
FIDRES 0.372529 Hz
AQ 1.3421773 sec
RG 501.187
DW 20.480 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D31 0.00001500 sec
D40 0.00439029 sec
L4 37
L5 53
P32 98.00 usec
TD0 14

======== CHANNEL f1 ========
SFO1 75.4828392 MHz
NUC1 13C
P1 15.00 usec
PLW1 22.00000000 W

======== CHANNEL f2 ========
SFO2 300.1612006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 98.00 usec
PLW2 9.30000019 W
PLW12 0.29359001 W
PLW13 0.20359001 W

F2 - Processing parameters
SI 32768
SF 75.4753350 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(4-acetamidophenyl)propanamide (5t)



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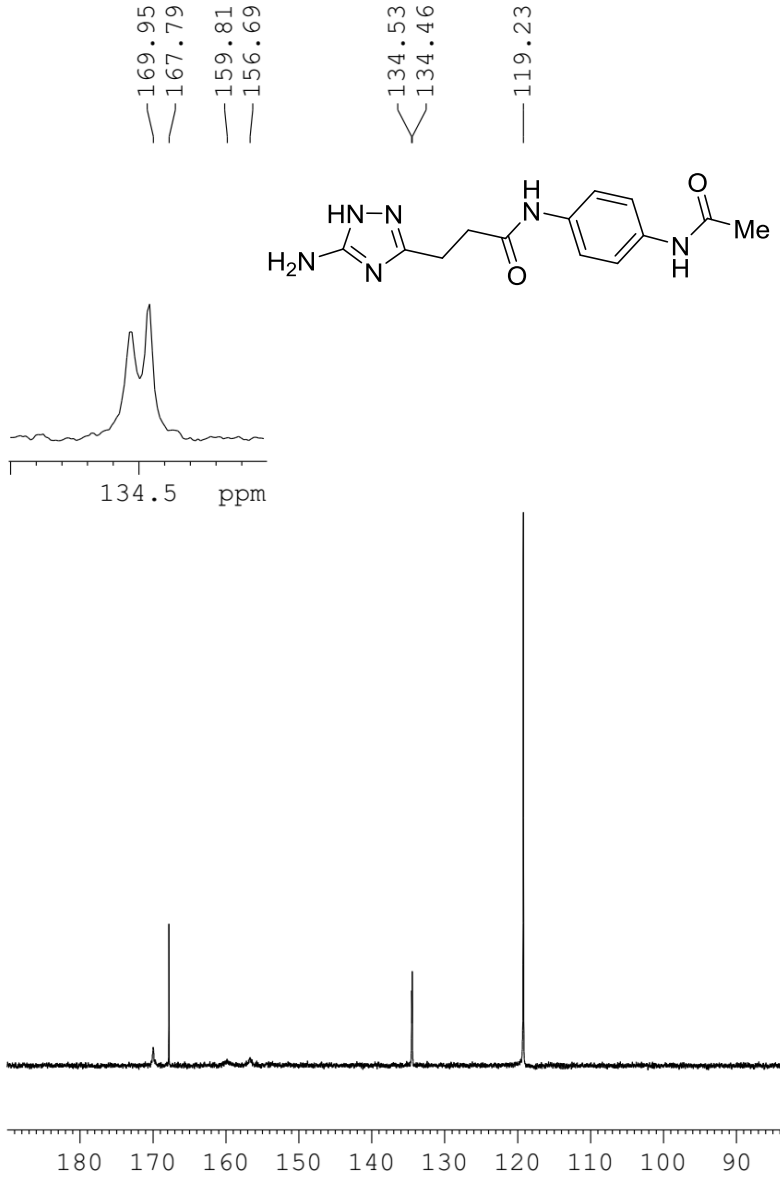
```
Current Data Parameters
NAME                  LY131
EXPNO                     3
PROCNO                    1

F2 - Acquisition Parameters
Date_              20171226
Time                  16.22
INSTRUM         FOURIER300
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       16
DS                        2
SWH                6103.516 Hz
FIDRES             0.093132 Hz
AQ                 5.3687091 sec
RG                   137.747
DW                    81.920 usec
DE                     6.50 usec
TE                    300.0 K
D1                 1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1            300.1618536 MHz
NUC1                      1H
P1                     13.50 usec
PLW1            9.30000019 W

F2 - Processing parameters
SI                    65536
SF              300.1600008 MHz
WDW                      EM
SSB       0
LB                     0.30 Hz
GB        0
PC                     1.00
```

3-(5-Amino-1H-1,2,4-triazol-3-yl)-N-(4-acetamidophenyl)propanamide (5t)



BRUKER

```
Current Data Parameters
NAME                 LY131
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20171213
Time                 19.48
INSTRUM       FOURIER300
PROBHD   5 mm DUL 13C-1
PULPROG           zgpg30
TD                 65536
SOLVENT              DMSO
NS                 14336
DS                     4
SWH            24414.063 Hz
FIDRES             0.372529 Hz
AQ                 1.3421773 sec
RG                   501.187
DW                  20.480 usec
DE                   6.50 usec
TE                  300.1 K
D1                 2.00000000 sec
D11                0.03000000 sec
D31                0.00001500 sec
D40                0.00439029 sec
L4                      37
L5                      53
P32                 98.00 usec
TD0                     14

======== CHANNEL f1 ========
SFO1            75.4828392 MHz
NUC1                   13C
P1                  15.00 usec
PLW1           22.00000000 W

======== CHANNEL f2 ========
SFO2           300.1612006 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2               98.00 usec
PLW2            9.30000019 W
PLW12           0.29359001 W
PLW13           0.20359001 W

F2 - Processing parameters
SI                     32768
SF              75.4753348 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

X-ray crystallography: packing and interactions in the crystals of 5j

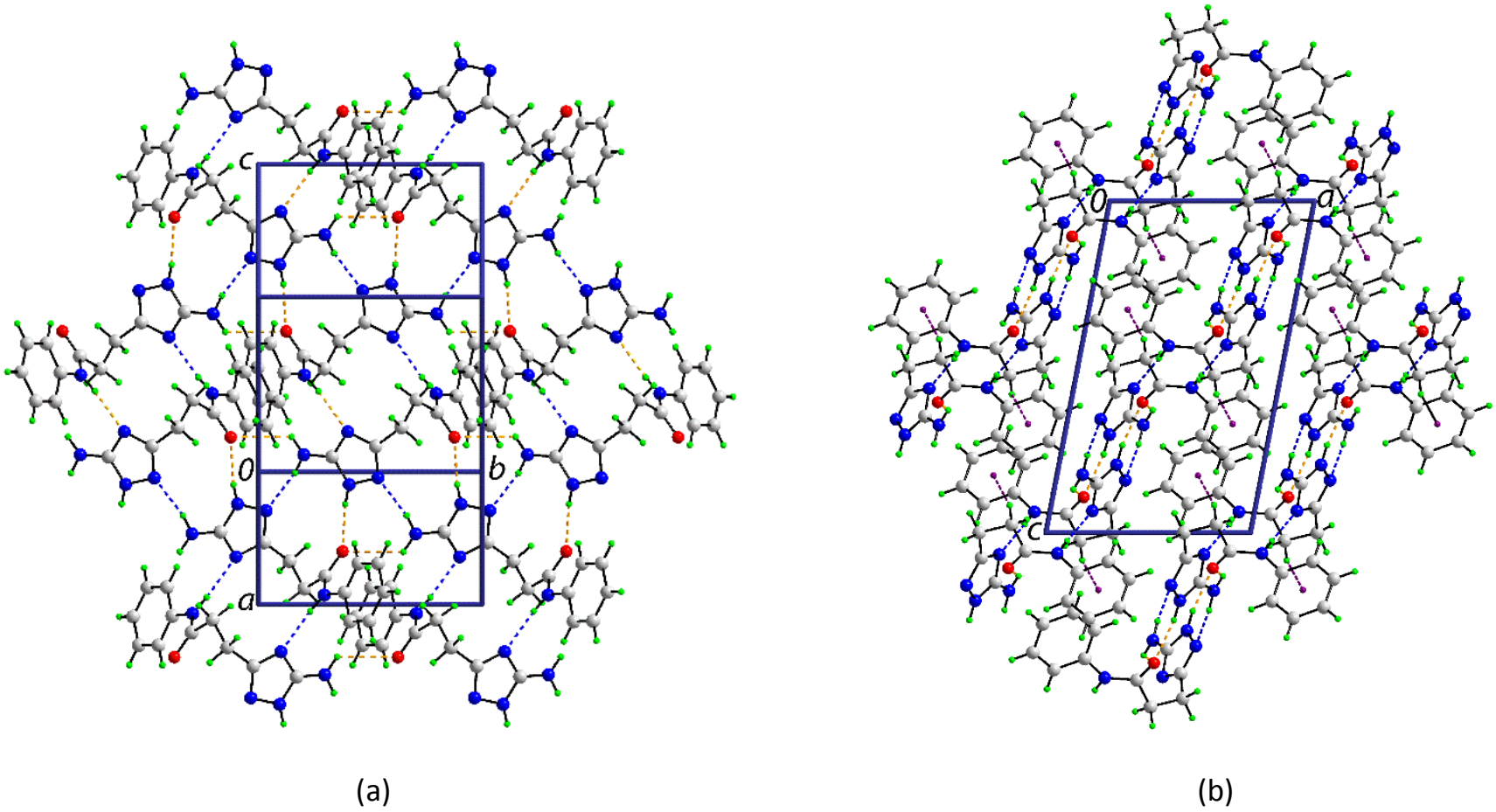


Figure S1. Molecular packing in **5j**: (a) a view of the supramolecular layer parallel to (1 0 1) sustained by N–H···O and N–H···N hydrogen bonding shown as orange and blue dashed lines, respectively, and (b) a view in projection down the *b*-axis of the unit cell contents. The C–H···π interactions are shown as purple dashed lines.

Table S1. Geometric parameters (Å, °) characterising the identified intermolecular interactions in the crystal of **5j**.

A	H	B	A–H	H···B	A···B	A–H···B	symm. operation
N1	H1n	O8	0.874(10)	1.994(11)	2.8568(13)	169.0(14)	½-x, ½+y, 1½-z
N5	H2n	N2	0.906(13)	1.998(14)	2.8866(15)	166.5(14)	½-x, ½+y, 1½-z
N5	H3n	O8	0.891(15)	2.535(15)	3.1243(14)	124.2(12)	x, 1+y, z
N8	H4n	N4	0.875(13)	2.038(13)	2.9106(14)	174.5(12)	1-x, 1-y, 1-z
C7	H7a	Cg(1)*	0.99	2.77	3.6701(12)	151	1-x, -y, 1-z

Cg(1) is the ring centroid of the C9-C14 ring.